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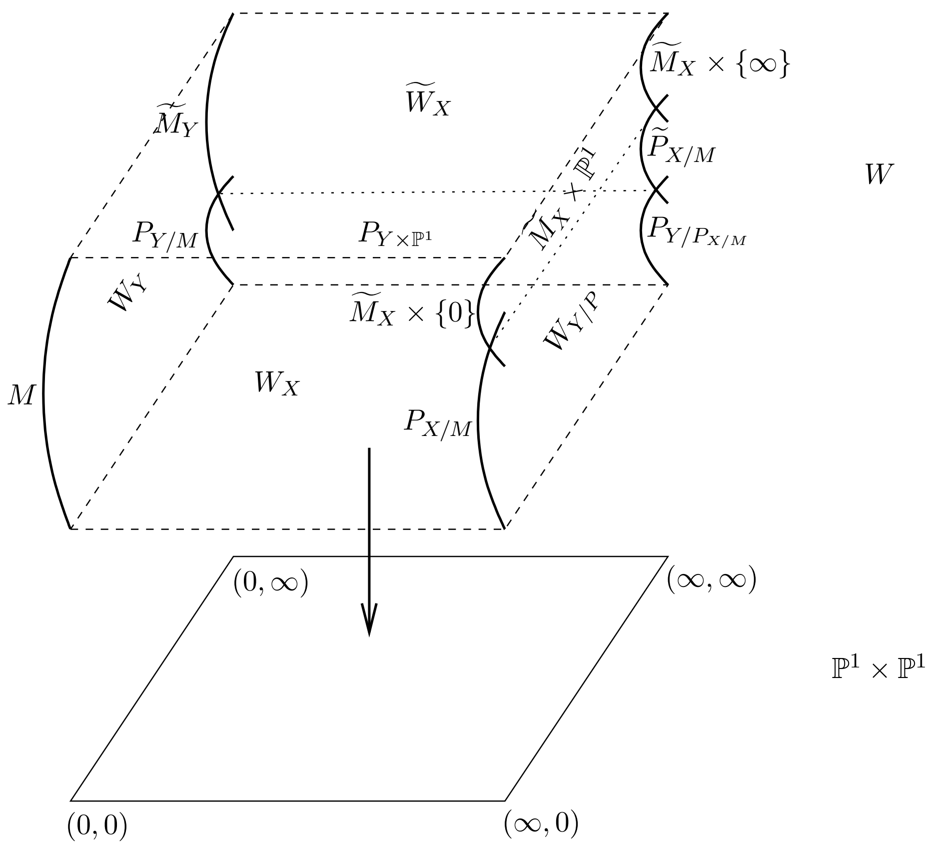

Figure 1. Double deformation, cf. page 131

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Standard Relations of Multiple Polylogarithm Values at Roots of Unity

Dedicated to Prof. Keqin Feng on his 70th birthday

Jianqiang Zhao

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Abstract. Let N be a positive integer. In this paper we shall study the special values of multiple polylogarithms at Nth roots of unity, called multiple polylogarithm values (MPVs) of level N. Our primary goal in this paper is to investigate the relations among the MPVs of the same weight and level by using the regularized double shuffle relations, regularized distribution relations, lifted versions of such relations from lower weights, and weight one relations which are produced by relations of weight one MPVs. We call relations from the above four families *standard*. Let $d(w,N)$ be the dimension of the $\mathbb{Q}$-vector space generated by all MPVs of weight w and level N. Recently Deligne and Goncharov were able to obtain some lower bound of $d(w,N)$ using the motivic mechanism. We call a level N *standard* if $N=1,2,3$ or $N=p^n$ for prime $p\ge 5$. Our computation suggests the following dichotomy: If N is standard then the standard relations should produce all the linear relations and if further $N>3$ then the bound of $d(w,N)$ by Deligne and Goncharov can be improved; otherwise there should be non-standard relations among MPVs for all sufficiently large weights (depending only on N) and the bound by Deligne and Goncharov may be sharp. We write down some of the non-standard relations explicitly with good numerical verification. In two instances ($N=4$, $w=3,4$) we can rigorously prove these relations by using the octahedral symmetry of $\{0,\infty,\pm 1,\pm\sqrt{-1}\}$. Throughout the paper we provide many conjectures which are strongly supported by computational evidence.

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Keywords and Phrases: Multiple polylogarithms, double shuffle relations, distribution relations, regularization, standard relations.

Contents

1 Introduction

In recent years, there is a revival of interest in multi-valued classical polylogarithms (polylogs) and their generalizations. For any positive integers $s_1, \dots, s_\ell$, multiple polylogs of complex variables are defined as follows (note that our index order is opposite to that of [19]):

$$Li_{s_1,\dots,s_\ell}(x_1, \dots, x_\ell) = \sum_{k_1 > \dots > k_\ell > 0} \frac{x_1^{k_1} \cdots x_\ell^{k_\ell}}{k_1^{s_1} \cdots k_\ell^{s_\ell}}, \tag{1}$$

where $|x_1 \cdots x_j| < 1$ for $j = 1, \dots, \ell$. It can be analytically continued to a multi-valued meromorhpic function on $\mathbb{C}^\ell$ (see [29]). Conventionally ℓ is called the *depth* (or *length*) and $s_1 + \cdots + s_\ell$ the *weight*. When the depth $\ell = 1$ the function is nothing but the classical polylog. When the weight is also 1 one gets the MacLaurin series of $-\log(1-x)$. Moreover, setting $x_1 = \cdots = x_\ell = 1$ and $s_1 > 1$ one obtains the well-known multiple zeta values (MZVs). If one allows x_j's to be ± 1 then one gets the so-called alternating Euler sums.

1.1 Multiple polylog values at roots of unity

In this paper, the primary objects of study are the multiple polylog values at roots of unity (MPVs). These special values, MZVs and the alternating Euler sums in particular, have attracted a lot attention in recent years after they were found to be connected to many branches of mathematics and physics (see, for e.g., [7, 8, 10, 11, 15, 19, 28]). Results up to around year 2000 can be found in the comprehensive survey paper [6].

Starting from early 1990s Hoffman [21, 22] has constructed some quasi-shuffle (called *stuffle* in [6]) algebras reflecting the essential combinatorial properties of MZVs. Later he [23] extends this to incorporate MPVs although his definition of $*$-product is different from ours. This approach was then improved in [24] and [26] to study MZVs and MPVs in general, respectively, where the regularized double shuffle relations play prominent roles. One derives these relations by comparing (1) with another expression of the multiple polylogs given by the following iterated integral:

$$Li_{s_1,\dots,s_\ell}(x_1,\dots,x_\ell) = \\ (-1)^\ell \int_0^1 \left(\frac{dt}{t}\right)^{\circ(s_1-1)} \circ \frac{dt}{t-a_1} \circ \cdots \circ \left(\frac{dt}{t}\right)^{\circ(s_\ell-1)} \circ \frac{dt}{t-a_\ell}, \quad (2)$$

where $a_i = 1/(x_1 \dots x_i)$ for $1 \le i \le \ell$. Here, one defines the iterated integrals recursively by $\int_a^b f(t) \circ w(t) = \int_a^b (\int_a^x w(t)) f(x)$ for any 1-form $w(t)$ and concatenation of 1-forms $f(t)$. One may think the path lies in $\mathbb{C}$; however, it is more revealing to use iterated integrals in $\mathbb{C}^\ell$ to find the analytic continuation of this function (see [29]).

The main feature of this paper is a quantitative comparison between the results obtained by Racinet [26] who considers MPVs from the motivic viewpoint of Drinfeld associators, and those by Deligne and Goncharov [17] who study the motivic fundamental groups of $\mathbb{P}^1 - (\{0,\infty\} \cup \boldsymbol{\mu}_N)$ by using the theory of mixed Tate motives over S-integers of number fields, where $\boldsymbol{\mu}_N$ is the group of Nth roots of unity.

Fix an Nth root of unity $\mu = \mu_N := \exp(2\pi\sqrt{-1}/N)$. An MPV of *level* N is a number of the form

$$L_N(s_1,\dots,s_\ell | i_1,\dots,i_\ell) := Li_{s_1,\dots,s_\ell}(\mu^{i_1},\dots,\mu^{i_\ell}). \quad (3)$$

We will always identify $(i_1,\dots,i_\ell)$ with $(i_1,\dots,i_\ell) \pmod N$. It is easy to see from (1) that an MPV converges if and only if $(s_1,\mu^{i_1}) \ne (1,1)$. Clearly, all

MPVs of level N are automatically of level Nk for every positive integer k. For example when $i_1 = \cdots = i_\ell = 0$ or $N = 1$ one gets the MZV $\zeta(s_1, \dots, s_\ell)$. When $N = 2$ one recovers the alternating Euler sums studied in [8, 31]. To save space, if a string S repeats n times then $\{S\}^n$ will be used. For example, $L_N(\{2\}^2|\{0\}^2) = \zeta(2,2) = \pi^4/120$.

Standard conjectures in arithmetic geometry imply that $\mathbb{Q}$-linear relations among MVPs can only exist between those of the same weight. Let $\mathcal{MPV}(w, N)$ be the $\mathbb{Q}$-span of all the MPVs of weight w and level N. Let $d(w, N)$ denoted its dimension. In general, it is very difficult to determine $d(w, N)$ because any nontrivial lower bound would provide some nontrivial irrational/transcendental result which is related to a variant of Grothendieck's period conjecture (see [16] or [17, 5.27(c)]). For example, one can show easily that $\mathcal{MPV}(2, 4) = \langle \log^2 2, \pi^2, \pi \log 2\sqrt{-1}, (K-1)\sqrt{-1}\rangle$, where $K = \sum_{n\geq 0}(-1)^n/(2n+1)^2$ is the Catalan's constant. From a variant of Grothendieck's period conjecture we know $d(2, 4) = 4$ (see [16]) but we don't have an unconditional proof yet. Namely, we cannot prove that the four number $\log^2 2, \pi^2, \pi \log 2\sqrt{-1}, (K-1)\sqrt{-1}$ are linearly independent over $\mathbb{Q}$. Thus, nontrivial lower bound of $d(w, N)$ is hard to come by.

On the other hand, one may obtain upper bound of $d(w, N)$ by finding as many linear relations in $\mathcal{MPV}(w, N)$ as possible. As in the cases of MZVs and the alternating Euler sums the double shuffle relations play important roles in revealing the relations among MPVs. In such a relation if all the MPVs involved are convergent it is called a *finite double shuffle relation* (FDS). In general one needs to use regularization to obtain *regularized double shuffle* relations (RDS) involving divergent MPVs. We shall recall this theory in §2 building on the results of [24, 26].

From the point of view of Lyndon words and quasi-symmetric functions Bigotte et al. [3, 4] have studied MPVs (they call them *colored MZVs*) primarily by using double shuffle relations and monodromy argument (cf. [4, Thm. 5.1]). However, when the level $N \geq 2$, these double shuffle relations often are not complete, as we shall see in this paper (for level two, see also [5]).

1.2 Standard relations of MPVs

If the level $N > 3$ then there are many non-trivial linear relations in $\mathcal{MPV}(1, N)$ of weight one whose structure is clear to us. Multiplied by MPVs of weight $w-1$ these relations can produce non-trivial linear relations among MPVs of weight w which are called the *weight one relations.* Similar to these relations one may produce new relations by multiplying MPVs on all of the other types of relations among MPVs of lower weights. We call such relations *lifted relations.*

It is well-known that among MPVs there are the so-called *finite distribution relations* (FDT), see (14). Racinet [26] further considers the regularization of these relations by regarding MPVs as the coefficients of some group-like element in a suitably defined pro-Lie-algebra of motivic origin (see §4). Our computation shows that the *regularized distribution relations* (RDT) do contribute to new relations not covered by RDS and FDT. But they are not enough yet to produce all the lifted RDS.

Definition 1.1. We call a $\mathbb{Q}$-linear relation between MPVs *standard*[1] if it can be produced by some $\mathbb{Q}$-linear combinations of the following four families of relations: regularized double shuffle relations (RDS), regularized distribution relations (RDT), weight one relations, and lifted relations from the above. Otherwise, it is called a *non-standard* relation.

It is commonly believed that all linear relations among MPVs (i.e. levels one MPVs) are consequences of RDS. When level $N = 2$ we believe that all linear relations among the alternating Euler sums are consequences of RDS and RDT. Further, in this case, the RDT should correspond to the doubling and generalized doubling relations of [5].

1.3 Main results

The main goal of this paper is to provide some extensive numerical evidence concerning the (in)completeness of the standard relations. Namely, these relations in general are not enough to produce all the $\mathbb{Q}$-linear relation between MPVs (see Remark 8.2 and Conjecture 8.5); however, we have the following result (see Thm. 8.6 and Thm. 8.3).

Theorem 1.2. *Let $p \geq 5$ be a prime. Then $d(2,p) \leq (5p+7)(p+1)/24$ and $d(2,p^2) < (p^2-p+2)^2/4$. If a variant of Grothendieck's period conjecture* [17, 5.27(c)] *is true then the equality holds for $d(2,p)$ and the standard relations in $\mathcal{MPV}(2,p)$ imply all the others.*

If weight $w = 2$ and $N = 5^2, 7^2, 11^2, 13^2$ or 5^3, then our computation (see Table 1) shows that the standard relations are very likely to be complete. However, if $N > 3$ is a 2-power or 3-power or has at least two distinct prime factors then the standard relations are often incomplete. Moreover, we don't know how to obtain the non-standard relations rigorously except that when the level $N = 4$ we get (see Thm. 9.1)

Theorem 1.3. *If the conjecture in* [17, 5.27(c)] *is true then all the linear relations among MPVs of level four and weight three (resp. weight four) are the consequences of the standard relations and the octahedral relation* (53) *(resp. the five octahedral relations* (54)-(58)*).*

Most of the MPV identities in this paper are discovered with the help of MAPLE using symbolic computations. We have verified all relations numerically by GiNaC [27] with an error bound $< 10^{-90}$. Some results contained in this paper were announced in [30].

[1] This term was suggested by P. Deligne in a letter to Goncharov and Racinet dated Feb. 25, 2008.

1.4 Acknowledgment

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2 The double shuffle relations and the algebra $\mathfrak{A}$

In this section we recall the procedure to transform the shuffle relations among MPVs into some pure algebra structures. This is a rather straight-forward variation of a theme first studied by Hoffman for MZVs (see, for e.g., [22, 23]) and then further developed by Ihara et al. in [24] and by Racinet in [26]. Most of the results in this section are well-known but we include them for the convenience of the reader.

It is Kontsevich [25] who first noticed that MZVs can be represented by iterated integrals. One can easily extend this to MPVs [26]. Set

$$a = \frac{dt}{t}, \qquad b_i = \frac{\mu^i dt}{1-\mu^i t} \quad \text{for } i = 0, 1, \dots, N-1.$$

For every positive integer n define the word of length n

$$y_{n,i} := a^{n-1} b_i.$$

Then it is straight-forward to verify using (2) that if $(s_1, \mu^{i_1}) \neq (1, 1)$ then (cf. [26, (2.5)])

$$L_N(s_1, \dots, s_n | i_1, i_2, \dots, i_n) = \int_0^1 y_{s_1,i_1} y_{s_2,i_1+i_2} \cdots y_{s_n,i_1+i_2+\cdots+i_n}. \qquad (4)$$

One can now define an algebra of words as follows:

Definition 2.1. Set $A_0 = \{\mathbf{1}\}$ to be the set of the empty word. Define $\mathfrak{A} = \mathbb{Q}\langle A\rangle$ to be the graded noncommutative polynomial $\mathbb{Q}$-algebra generated by letters a and b_i for $i \equiv 0, \dots, N-1 \pmod N$, where A is a locally finite set of generators whose degree n part A_n consists of words (i.e., a monomial in the letters) of depth n. Let $\mathfrak{A}^0$ be the subalgebra of $\mathfrak{A}$ generated by words not beginning with b_0 and not ending with a. The words in $\mathfrak{A}^0$ are called *admissible words.*

Observe that every MPV can be expressed as an iterated integral over the closed interval $[0,1]$ of an admissible word w in $\mathfrak{A}^0$. This is denoted by

$$Z(w) := \int_0^1 w. \tag{5}$$

We remark that the length $\lg(w)$ of w is equal to the weight of $Z(w)$. Therefore in general one has (cf. [26, (2.5) and (2.6)])

$$L_N(s_1,\dots,s_n|i_1,i_2,\dots,i_n) = Z(y_{s_1,i_1}y_{s_2,i_1+i_2}\cdots y_{s_n,i_1+i_2+\cdots+i_n}), \tag{6}$$
$$Z(y_{s_1,i_1}y_{s_2,i_2}\cdots y_{s_n,i_n}) = L_N(s_1,\dots,s_n|i_1,i_2-i_1,\dots,i_n-i_{n-1}). \tag{7}$$

For example $L_3(1,2,2|1,0,2) = Z(y_{1,1}y_{2,1}y_{2,0})$. On the other hand, during 1960s Chen developed a theory of iterated integral which can be applied in our situation.

Lemma 2.2. ([12, (1.5.1)]) *Let ω_i $(i \ge 1)$ be $\mathbb{C}$-valued 1-forms on a manifold M. For every path p,*

$$\int_p \omega_1\cdots\omega_r \int_p \omega_{r+1}\cdots\omega_{r+s} = \int_p (\omega_1\cdots\omega_r)\,ш\,(\omega_{r+1}\cdots\omega_{r+s})$$

where ш is the shuffle product defined by

$$(\omega_1\cdots\omega_r)\,ш\,(\omega_{r+1}\cdots\omega_{r+s}) := \sum_{\substack{\sigma\in S_{r+s},\sigma^{-1}(1)<\cdots<\sigma^{-1}(r)\\ \sigma^{-1}(r+1)<\cdots<\sigma^{-1}(r+s)}} \omega_{\sigma(1)}\cdots\omega_{\sigma(r+s)}.$$

For example, one has

$$\begin{aligned} &L_N(1|1)L_N(2,3|1,2) = Z(y_{1,1})Z(y_{2,1}y_{3,3}) = Z(b_1\,ш\,(ab_1a^2b_3))\\ =&Z(b_1ab_1a^2b_3 + 2ab_1^2a^2b_3 + (ab_1)^2ab_3 + ab_1a^2b_1b_3 + ab_1a^2b_3b_1)\\ =&Z(y_{1,1}y_{2,1}y_{3,3} + 2y_{2,1}y_{1,1}y_{3,3} + y_{2,1}^2y_{2,3} + y_{2,1}y_{3,1}y_{1,3} + y_{2,1}y_{3,3}y_{1,1})\\ =&L_N(1,2,3|1,0,2) + 2L_N(2,1,3|1,0,2) + L_N(2,2,2|1,0,2)\\ &\qquad + L_N(2,3,1|1,0,2) + L_N(2,3,1|1,2,N-2). \end{aligned}$$

Let $\mathfrak{A}_ш$ be the algebra of $\mathfrak{A}$ together with the multiplication defined by shuffle product ш. Denote the subalgebra $\mathfrak{A}^0$ by $\mathfrak{A}^0_ш$ when one considers the shuffle product. Then one can easily prove

Proposition 2.3. *The map $Z : \mathfrak{A}^0_ш \longrightarrow \mathbb{C}$ is an algebra homomorphism.*

On the other hand, MPVs are known to satisfy the series stuffle relations. For example

$$L_N(2|5)L_N(3|4) = L_N(2,3|5,4) + L_N(3,2|4,5) + L_N(5|9).$$

To study such relations in general one has the following definition.

DEFINITION 2.4. Denote by $\mathfrak{A}^1$ the subalgebra of $\mathfrak{A}$ which is generated by words $y_{s,i}$ with $s \in \mathbb{N}$ and $i \equiv 0, \dots, N-1 \pmod N$. Equivalently, $\mathfrak{A}^1$ is the subalgebra of $\mathfrak{A}$ generated by words not ending with a. For any word $w = y_{s_1,i_1} y_{s_2,i_2} \cdots y_{s_n,i_n} \in \mathfrak{A}^1$ and positive integer j one defines the exponent shifting operator τ_j by

$$\tau_j(w) = y_{s_1,j+i_1} y_{s_2,j+i_2} \cdots y_{s_n,j+i_n}.$$

For convenience, on the empty word we adopt the convention that $\tau_j(\mathbf{1}) = \mathbf{1}$. We then define another multiplication $*$ on $\mathfrak{A}^1$ by requiring that $*$ distribute over addition, that $\mathbf{1} * w = w * \mathbf{1} = w$ for any word w, and that, for any words ω_1, ω_2,

$$y_{s,j}\omega_1 * y_{t,k}\omega_2 = y_{s,j}\Big(\tau_j\big(\tau_{-j}(\omega_1) * y_{t,k}\omega_2\big)\Big) + y_{t,k}\Big(\tau_k\big(y_{s,j}\omega_1 * \tau_{-k}(\omega_2)\big)\Big) + y_{s+t,j+k}\Big(\tau_{j+k}\big(\tau_{-j}(\omega_1) * \tau_{-k}(\omega_2)\big)\Big). \quad (8)$$

This multiplication is called the *stuffle product* in [6].

If one denotes by $\mathfrak{A}^1_*$ the algebra $(\mathfrak{A}^1, *)$ then it is not hard to show that

PROPOSITION 2.5. (cf. [22, Thm. 2.1]) *The polynomial algebra $\mathfrak{A}^1_*$ is a commutative graded $\mathbb{Q}$-algebra.*

Now one can define the subalgebra $\mathfrak{A}^0_*$ similar to $\mathfrak{A}^0_ш$ by replacing the shuffle product by the stuffle product. Then by induction on the lengths and using the series definition one can quickly check that for any $\omega_1, \omega_2 \in \mathfrak{A}^0_*$

$$Z(\omega_1)Z(\omega_2) = Z(\omega_1 * \omega_2).$$

This implies that

PROPOSITION 2.6. *The map $Z : \mathfrak{A}^0_* \longrightarrow \mathbb{C}$ is an algebra homomorphism.*

DEFINITION 2.7. Let w be a positive integer such that $w \geq 2$. For nontrivial $\omega_1, \omega_2 \in \mathfrak{A}^0$ with $\lg(\omega_1) + \lg(\omega_2) = w$ one says that

$$Z(\omega_1 ш \omega_2 - \omega_1 * \omega_2) = 0 \quad (9)$$

is a *finite double shuffle* relation (FDS) of weight w.

It is known that even in level one these relations are not enough to provide all the relations among MZVs. However, it is believed that one can remedy this by considering *regularized double shuffle* relation (RDS) produced by the following mechanism. This is explained in detail in [24] when Ihara, Kaneko and Zagier consider MZVs where they call these *extended double shuffle* relations or EDS. It is also contained in [26] with a different formulation.
To produce RDS, first, combining Propositions 2.6 and 2.3 one can easily prove the following algebraic result (cf. [24, Prop. 1]):

Proposition 2.8. *One has two algebra homomorphisms:*

$$Z^* : (\mathfrak{A}^1_*, *) \longrightarrow \mathbb{C}[T], \quad \textit{and} \quad Z^{ш} : (\mathfrak{A}^1_{ш}, ш) \longrightarrow \mathbb{C}[T]$$

which are uniquely determined by the properties that they both extend the evaluation map $Z : \mathfrak{A}^0 \longrightarrow \mathbb{C}$ *by sending* $b_0 = y_{1,0}$ *to* T.

Second, in order to establish the crucial relation between Z^* and $Z^{ш}$ one can adopt the machinery in [24] as follows. For any $(\mathbf{s}|\mathbf{i}) = (s_1, \dots, s_n|i_1, \dots, i_n)$ where i_j's are integers and s_j's are positive integers, let the image of the corresponding words in $\mathfrak{A}^1$ under Z^* and $Z^{ш}$ be denoted by $Z^*_{(\mathbf{s}|\mathbf{i})}(T)$ and $Z^{ш}_{(\mathbf{s}|\mathbf{i})}(T)$ respectively.

Theorem 2.9. (cf. [26, Cor. 2.24]) *Define a* $\mathbb{C}$*-linear map* $\rho : \mathbb{C}[T] \to \mathbb{C}[T]$ *by*

$$\rho(e^{Tu}) = \exp\left(\sum_{n=2}^{\infty} \frac{(-1)^n}{n} \zeta(n) u^n\right) e^{Tu}, \qquad |u| < 1.$$

Then for any index set $(\mathbf{s}|\mathbf{i})$ *one has*

$$Z^{ш}_{(\mathbf{s}|\mathbf{i})}(T) = \rho(Z^*_{(\mathbf{s}|\mathbf{i})}(T)). \tag{10}$$

Definition 2.10. Let w be a positive integer such that $w \geq 2$. Let $(\mathbf{s}|\mathbf{i})$ be any index set with the weight of $\mathbf{s}$ equal to w. Then every weight w MPV relation produced by (10) is called a *regularized double shuffle* relation (RDS) of weight w. This is obtained by formally setting $T = 0$ in (10).

Theorem 2.9 is a generalization of [24, Thm. 1] to the higher level MPV cases. The proof is essentially the same. The above steps can be easily transformed to computer codes which are used in our MAPLE programs. For example, one gets by stuffle product

$$\begin{aligned} TL_N(2|3) =& Z^*_{(1|0)}(T) Z^*_{(2|3)}(T) = Z^*(y_{1,0} * y_{2,3}) \\ =& Z^*_{(1,2|0,3)}(T) + Z^*_{(2,1|3,3)}(T) + Z^*_{(3|3)}(T), \end{aligned}$$

while using shuffle product one has

$$\begin{aligned} TL_N(2|3) =& Z^{ш}_{(1|0)}(T) Z^{ш}_{(2|3)}(T) = Z^{ш}(y_{1,0} ш y_{2,3}) = Z^{ш}(b_0 ш a b_3) \\ =& Z^{ш}_{(1,2|0,3)}(T) + Z^{ш}_{(2,1|0,3)}(T) + Z^{ш}_{(2,1|3,0)}(T). \end{aligned}$$

Hence one discovers the following RDS by comparing the above two expressions using Thm. 2.9:

$$L_N(2,1|3,0) + L_N(3|3) = L_N(2,1|3,N-3) + L_N(2,1|0,3).$$

3 Weight one relations

When $N \geq 4$ there exist linear relations among MPVs of weight one by a theorem of Bass [1]. These relations are important because by multiplying any MPV of weight $w-1$ by such a relation one can get a relation between MPVs of weight w which is called a *weight one relation.* This is one of the key ideas in finding the formula in [17, 5.25] concerning $d(w,N)$.
Clearly, there are $N-1$ MPVs of weight 1 and level N:

$$L_N(1|j) = -\log(1-\mu^j), \qquad 0<j<N,$$

where $\mu = \mu_N = \exp(2\pi\sqrt{-1}/N)$ as before. Here one can take $\mathbb{C} - (-\infty, 0]$ as the principle branch of the logarithm. Further, it follows from the motivic theory of classical polylogs developed by Beilinson and Deligne in [2] and the Borel's theorem (see [20, Thm. 2.1]) that the $\mathbb{Q}$-dimension of $\mathcal{MPV}(1,N)$ is

$$d(1,N) = \dim K_1(\mathbb{Z}[\mu_N][1/N]) \otimes \mathbb{Q} + 1 = \varphi(N)/2 + \nu(N),$$

where φ is the Euler's totient function and $\nu(N)$ is the number of distinct prime factors of N. Hence there are many linear relations among $L_N(1|j)$. For instance, if $j<N/2$ then one has the symmetric relation

$$-\log(1-\mu^j) = -\log(1-\mu^{N-j}) - \log(-\mu^j) = -\log(1-\mu^{N-j}) + \frac{N-2j}{N}\pi\sqrt{-1}.$$

Thus for all $1<j<N/2$

$$(N-2)(L_N(1|j) - L_N(1|N-j)) = (N-2j)(L_N(1|1) - L_N(1|N-1)). \quad (11)$$

Further, from [1, (B)] for any divisor d of N and $1 \leq a < N/d$ one has the distribution relation

$$\sum_{0\leq j<d} L_N(1|a+jN/d) = L_N(1|ad). \quad (12)$$

It follows from the main result of Bass [1] (corrected by Ennola [18]) that all the linear relations between $L_N(1|j)$ are consequences of (11) and (12). Hence the weight one relations have the following forms in words: for all $w \in \mathfrak{A}^0$

$$\begin{cases} (N-2)Z(y_{1,j} * w - y_{1,-j} * w) =(N-2j)Z(y_{1,1} * w - y_{1,-1} * w), \\ \displaystyle\sum_{0\leq j<d} Z(y_{1,a+jN/d} * w) =Z(y_{1,ad} * w). \end{cases} \quad (13)$$

4 Regularized distribution relations

It is well-known that multiple polylogs satisfy the following distribution formula (cf. [26, Prop. 2.25]):

$$Li_{s_1,\dots,s_n}(x_1,\dots,x_n) = d^{s_1+\dots+s_n-n} \sum_{y_j^d=x_j, 1\leq j\leq n} Li_{s_1,\dots,s_n}(y_1,\dots,y_n), \quad (14)$$

for all positive integer d. When $s_1 = 1$ one has to exclude the divergent case $x_1 = 1$. We call these *finite distribution relations* (FDT). Racinet further considers the regularized version of these relations, which we now recall briefly. Fix an embedding $\boldsymbol{\mu}_N \hookrightarrow \mathbb{C}$ and denote by Γ its image. Define two sets of words

$$\mathbf{X} := \mathbf{X}_\Gamma = \{x_\sigma : \sigma \in \Gamma \cup \{0\}\}, \quad \text{and} \quad \mathbf{Y} := \mathbf{Y}_\Gamma = \{x_0^{n-1} x_\sigma : n \in \mathbb{N}, \sigma \in \Gamma\}.$$

Then one may consider the coproduct Δ of $\mathbb{Q}\langle \mathbf{X} \rangle$ defined by $\Delta x_\sigma = 1 \otimes x_\sigma + x_\sigma \otimes 1$ for all $\sigma \in \Gamma \cup \{0\}$. For every path $\gamma \in \mathbb{P}^1(\mathbb{C}) - (\{0, \infty\} \cup \Gamma)$ Racinet defines the group-like element $\mathcal{I}_\gamma \in \mathbb{C}\langle\langle \mathbf{X} \rangle\rangle$ by

$$\mathcal{I}_\gamma := \sum_{p \in \mathbb{N}, \sigma_1, \ldots, \sigma_p \in \Gamma \cup \{0\}} \mathcal{I}_\gamma(\sigma_1, \ldots, \sigma_p) x_{\sigma_1} \cdots x_{\sigma_p},$$

where $\mathcal{I}_\gamma(\sigma_1, \ldots, \sigma_p)$ is the iterated integral $\int_\gamma \omega(\sigma_1) \cdots \omega(\sigma_p)$ with

$$\omega(\sigma)(t) = \begin{cases} \sigma \, dt/(1 - \sigma t), & \text{if } \sigma \neq 0; \\ dt/t, & \text{if } \sigma = 0. \end{cases}$$

(One has to correct the obvious typo in the displayed formula just before Prop. 2.8 in [26] by changing a_j to α_j.) This I_γ is essentially the same element denoted by dch in [17]. Note that $\mathbb{Q}\langle \mathbf{Y} \rangle$ is the sub-algebra of $\mathbb{Q}\langle \mathbf{X} \rangle$ generated by words not ending with x_0. Let $\pi_\mathbf{Y} : \mathbb{Q}\langle \mathbf{X} \rangle \to \mathbb{Q}\langle \mathbf{Y} \rangle$ be the projection. As x_0 is a primitive element one quickly deduces that $(\mathbb{Q}\langle \mathbf{Y} \rangle, \Delta)$ has a graded co-algebra structure.

Let $\mathbb{Q}\langle \mathbf{X} \rangle_{\mathsf{cv}}$ be the sub-algebra of $\mathbb{Q}\langle \mathbf{X} \rangle$ not beginning with x_1 and not ending with x_0. Let $\pi_{\mathsf{cv}} : \mathbb{Q}\langle \mathbf{X} \rangle \to \mathbb{Q}\langle \mathbf{X} \rangle_{\mathsf{cv}}$ be the projection. Passing to the limit one gets:

Proposition 4.1. ([26, Prop.2.11]) *The series* $\mathcal{I}_{\mathsf{cv}} := \lim_{a \to 0^+, b \to 1^-} \pi_{\mathsf{cv}}(\mathcal{I}_{[a,b]})$ *is group-like in* $(\mathbb{C}\langle\langle \mathbf{X} \rangle\rangle_{\mathsf{cv}}, \Delta)$.

Remark 4.2. The algebras $\mathfrak{A}$, $\mathfrak{A}^0$ and $\mathfrak{A}^1$ in §2 are essentially equal to $\mathbb{Q}\langle \mathbf{X} \rangle$, $\mathbb{Q}\langle \mathbf{X} \rangle_{\mathsf{cv}}$ and $\mathbb{Q}\langle \mathbf{Y} \rangle$, respectively, after setting $a = x_0$ and $b_j = x_{\mu^j}$.

Let $\mathcal{I}$ be the unique group-like element in $(\mathbb{C}\langle\langle \mathbf{X} \rangle\rangle, \Delta)$ whose coefficients of x_0 and x_1 are 0 such that $\pi_{\mathsf{cv}}(\mathcal{I}) = \mathcal{I}_{\mathsf{cv}}$. In order to do the numerical computation one needs to determine explicitly the coefficients for $\mathcal{I}$. Put

$$\mathcal{I} = \sum_{p \in \mathbb{N},, \sigma_1, \ldots, \sigma_p \in \Gamma \cup \{0\}} C(\sigma_1, \ldots, \sigma_p) x_{\sigma_1} \cdots x_{\sigma_p}. \tag{15}$$

Proposition 4.3. *Let* p, m *and* n *be three non-negative integers. If* $p > 0$ *then* *we assume* $\sigma_1 \neq 1$ *and* $\sigma_p \neq 0$. *Set* $(\sigma_1, \dots, \sigma_p, \{0\}^n) = (\sigma_1, \dots, \sigma_q)$. *Then*

$$C(\{1\}^m, \sigma_1, \dots, \sigma_p, \{0\}^n)$$
$$= \begin{cases} 0, & \text{if } mn = p = 0; \\ Z\big(\pi_{\mathsf{cv}}(x_{\sigma_1} \cdots x_{\sigma_p})\big), & \text{if } m = n = 0; \\ -\dfrac{1}{m} \displaystyle\sum_{i=1}^{q} C(\{1\}^{m-1}, \sigma_1, \dots, \sigma_i, 1, \sigma_{i+1}, \dots, \sigma_q), & \text{if } m > 0; \\ -\dfrac{1}{n} \displaystyle\sum_{i=1}^{p} C(\sigma_1, \dots, \sigma_{i-1}, 0, \sigma_i, \dots, \sigma_p, \{0\}^{n-1}), & \text{if } m = 0, n > 0. \end{cases} \tag{16}$$

Here Z *is defined by* (5) *after using the identification given by Remark* 4.2.

Remark 4.4. This proposition provides the recursive relations one may use to compute all the coefficients of $\mathcal{I}$.

Proof. Since $\mathcal{I}$ is group-like one has

$$\Delta \mathcal{I} = \mathcal{I} \otimes \mathcal{I}. \tag{17}$$

The first case follows from this immediately since $C(0) = C(1) = 0$. The second case is essentially the definition (5) of Z. If $m > 0$ then one can compare the coefficient of $x_1 \otimes x_1^{m-1} x_{\sigma_1} \cdots x_{\sigma_q}$ of the two sides of (17) and find the relation (16). Finally, if $m = 0$ and $n > 0$ then one may similarly consider the coefficient of $x_{\sigma_1} \cdots x_{\sigma_p} x_0^{n-1} \otimes x_0$ in (17). This finishes the proof of the proposition. □

For any divisor d of N let $\Gamma^d = \{\sigma^d : \sigma \in \Gamma\}$, $i_d : \Gamma^d \hookrightarrow \Gamma$ the embedding, and $p^d : \Gamma \twoheadrightarrow \Gamma^d$ the dth power map. They induce two algebra homomorphisms:

$$p^d_* : \mathbb{Q}\langle \mathbf{X}_\Gamma \rangle \longrightarrow \mathbb{Q}\langle \mathbf{X}_{\Gamma^d} \rangle$$
$$x_\sigma \longmapsto \begin{cases} dx_0, & \text{if } \sigma = 0, \\ x_{\sigma^d}, & \text{if } \sigma \in \Gamma, \end{cases}$$

and

$$i^*_d : \mathbb{Q}\langle \mathbf{X}_\Gamma \rangle \longrightarrow \mathbb{Q}\langle \mathbf{X}_{\Gamma^d} \rangle$$
$$x_\sigma \longmapsto \begin{cases} x_0, & \text{if } \sigma = 0, \\ x_\sigma, & \text{if } \sigma \in \Gamma^d, \\ 0, & \text{otherwise.} \end{cases}$$

It is easy to see that both i^*_d and p^d_* are Δ-coalgebra morphisms such that $i^*_d(\mathcal{I})$ and $p^d_*(\mathcal{I})$ have the same image under the map π_{cv}. By the standard Lie-algebra mechanism one has

Proposition 4.5. ([26, Prop.2.26]) *For every divisor d of N*

$$p_*^d(\mathcal{I}) = \exp\left(\sum_{\sigma^d=1,\sigma\neq 1} Li_1(\sigma)x_1\right) i_d^*(\mathcal{I}). \tag{18}$$

Combined with Proposition 4.3 the above result provides the so-called *regularized distribution relations* (RDT) which of course include all the FDT of MPVs given by (14).

However, sometimes FDT are not independent of the other relations. In the next theorem one sees that when the weight $w = 2$ and level N is a prime, all the distribution relations in (14), where $x_j = 1$ for all j, are consequences of RDS of MPVs of level N.

Theorem 4.6. *For any prime p write $L(i,j) = L_p(1,1|i,j)$ and $D(i) = L_p(2|i)$. Define for $1 \le i,j < p$:*

$$\text{FDT} := -D(0) + p\sum_{j=0}^{p-1} D(j), \qquad \text{RDS}(i) := D(i) + L(i,0) - L(i,-i),$$
$$\text{FDS}(i,j) := D(i+j) + L(i,j) + L(j,i) - L(i,j-i) - L(j,i-j).$$

Then one has

$$\text{FDT} = \sum_{1\le i<p} \text{FDS}(i,i) + 2\sum_{1\le j<i<p} \text{FDS}(i,j) + 2\sum_{i=1}^{p-1} \text{RDS}(i). \tag{19}$$

Proof. When $p = 2$ the second term on the right hand side of (19) is vacuous. Then it is easy to see that both sides of (19) are equal to $D(0) + 2D(1)$.

We now assume $p \ge 3$. Changing the order of summation yields that

$$\begin{aligned}
2\sum_{1\le j<i<p} D(i+j) &= \sum_{i=2}^{p-1}\sum_{j=1}^{i-1} D(i+j) + \sum_{j=1}^{p-2}\sum_{i=j+1}^{p-1} D(i+j)\\
&=\sum_{i=2}^{p-2}\sum_{i\neq j=1}^{p-1} D(i+j) + \sum_{j=1}^{p-2} D(j-1) + \sum_{i=2}^{p-1} D(i+1)\\
&=(p-3)\sum_{j=0}^{p-1} D(j) - \sum_{i=2}^{p-2} D(i) - \sum_{i=1}^{p-1} D(2i) + \sum_{j=1}^{p-2} D(j) + \sum_{j=2}^{p-1} D(j) + 2D(0)\\
&=(p-1)D(0) + (p-3)\sum_{j=1}^{p-1} D(j)
\end{aligned}$$

since $\sum_{j=0}^{p-1} D(i+j) = \sum_{j=0}^{p-1} D(j)$ for all i and $\sum_{i=1}^{p-1} D(2i) = \sum_{i=1}^{p-1} D(i)$. This implies that the dilogarithms on the right hand side of (19) exactly add up to

FDT. Thus one only needs to show that all the double logarithms on the right hand side of (19) cancel out.

First observe that $L(i,0)$ in FDS(i,i) and RDS(i) cancel out each other. Now let us consider the lattice points (i,j) of $\mathbb{Z}^2$ corresponding to $L(i,j)$. The points (i,j) corresponding to $L(i,j)$ with positive signs fill in exactly the area inside the square $[1,p-1]\times[1,p-1]$ (including boundary): $L(i,i)$ in FDS(i,i) provides the diagonal $y=x$, $\sum_{1\le j<i<p} L(i,j)$ (resp. $\sum_{1\le j<i<p} L(j,i)$) form the lower right (resp. upper left) triangular region.

For the negative terms of the double logs, $L(i,-i)$ in RDS(i) provides the diagonal $x+y=p$, $\sum_{1\le j<i<p} L(i,j-i)=\sum_{i=2}^{p-1}\sum_{j=p+1-i}^{p-1} L(i,j)$ form the upper right triangular region. Similarly, by changing the order of summation $\sum_{1\le j<i<p} L(j,i-j)=\sum_{i=1}^{p-2}\sum_{j=i+1}^{p-1} L(i,j-i)=\sum_{i=1}^{p-2}\sum_{j=1}^{p-1-i} L(i,j)$ fills the lower left region. □

To conclude this section we remark that numerical evidence up to level $N=169$ supports the following

Conjecture 4.7. *In weight two, all RDT are consequences of the weight one relations, RDS and depth two FDT.*

5 Lifted relations from lower weights

Note that when $N=3$ there are no weight one relations nor (regularized) distribution relations. When we deal with MZVs (resp. alternating Euler sums) we expect that all the linear relations come from RDS (resp. RDS and RDT). Since there is no weight one relation when level $N\le 3$ it is natural to ask if RDS and RDT are enough when $N=3$. Surprisingly, the answer is no.

The first counterexample is in weight four, i.e., $(w,N)=(4,3)$. Easy computation shows that there are 144 MPVs in this case among which there are 239 nontrivial RDS of weight four which include 191 FDS of weight four (see (9) and (10)). Furthermore, it is easy to verify that all the seven RDT (including four FDT) can be derived from RDS. Using these relations we get 127 independent linear relations among the 144 MPVs. But we have $d(4,3)\le 16$ by [17, 5.25], so there must be at least one more linearly independent relation. Where else can we find it? The answer is the so-called *lifted relations.*.

We know that a product of two weight two MPVs is of weight four. So on each of the five RDS (including two FDS) of weight two in $\mathcal{MPV}(2,3)$ we can multiply any one of the nine MPVs of $(w,N)=(2,3)$ to get a relation in $\mathcal{MPV}(4,3)$. For instance, we have a FDS

$$Z(y_{1,1}*y_{1,1}-y_{1,1}ш y_{1,1})=L_3(2|2)+2L_3(1,1|1,1)-L_3(1,1|1,0)=0.$$

Multiplying by $L_3(1,1|1,1)=Z(y_{1,1}y_{1,2})$ we obtain a new relation which is linearly independent from RDS of weight four in $\mathcal{MPV}(4,3)$:

$$\begin{aligned}&Z\big(y_{1,1}y_{1,2}ш(y_{2,0}+2y_{1,1}y_{1,2}-2y_{1,1}y_{1,0})\big)\\ =&L_3(1,1,2|1,1,0)+2L_3(1,2,1|1,1,0)+2L_3(2,1,1|1,1,0)\\ +&L_3(2,1,1|2,2,1)+4L_3(\{1\}^4|1,1,2,1)+8L_3(\{1\}^4|1,0,1,0)\\ -&6L_3(\{1\}^4|1,0,0,1)-4L_3(\{1\}^4|1,0,1,2)-2L_3(\{1\}^4|1,1,2,0)=0.\end{aligned}$$

Such relations coming from the lower weights are called *lifted relations.* In this way, when $(w,N)=(4,3)$ we can produce 45 lifted RDS relations from weight two, 58 from weight three. We may also lift RDT and obtain nine and six relations from weight two and three, respectively. However, all the lifted relations together only produce one new linearly independent relation, as expected. Hence we find totally 128 linearly independent relations among the 144 MPVs with $(w,N)=(4,3)$. This implies that $d(4,3)\le 16$ which is the same bound obtained by [17, 5.25] and is proved to be exact under a variant of Grothendieck's period conjecture by Deligne [16].
For levels $N\ge 4$ one may lift not only RDS and RDT but also the weight one relations. But by a moment reflection one sees that the lifted weight one relations are still weight one relations by themselves so one doesn't really need to consider them after all.

Definition 5.1. We call a $\mathbb{Q}$-linear relation among MPVs *standard* if it can be produced by some $\mathbb{Q}$-linear combinations of the following four families of relations: regularized double shuffle relations, regularized distribution relations, weight one relations, and lifted relations from the above. Otherwise, it is called a *non-standard* relation.

In general, there are no inclusion relations among the four families of the standard relations.
Computation in small weight cases supports the following

Conjecture 5.2. *Suppose $N=3$ or 4. Every MPV of level N is a linear combination of MPVs of the form $L(\{1\}^w|t_1,\dots,t_w)$ with $t_j\in\{1,2\}$. Consequently, the $\mathbb{Q}$-dimension of the MPVs of weight w and level N is given by $d(w,N)=2^w$ for all $w\ge 1$.*

Remark 5.3. The data in Table 2 in §7 shows that one cannot produce enough relations by using only the standard relations when $(w,N)=(3,4)$. In fact, even though one has $d(3,4)\le 8$ and $d(4,4)\le 16$ by [17, 5.25], one can only show that $d(3,4)\le 9$ and $d(4,4)\le 21$ by using only the standard relations. However, thanks to the octahedral symmetry of $\mathbb{P}^1-(\{0,\infty\}\cup\boldsymbol{\mu}_4)$ one can find (presumably all) the non-standard relations in these two cases (see Thm. 9.1).

Remark 5.4. Let $N=2,3,4$ or 8. Assuming a variant of Grothendieck's period conjecture, Deligne [16] constructed explicitly a set of basis for $\mathcal{MPV}(w,N)$. His results would also imply that $d(w,2)$ is given by the Fibonacci numbers, $d(w,3)=d(w,4)=2^w$, and $d(w,8)=3^w$ under Grothendieck's period conjecture.

6 Some conjectures of FDS and RDS

Fix a level N. Let R be a commutative $\mathbb{Q}$-algebra with 1 and a homomorphism $Z_R : \mathfrak{A}^0 \longrightarrow R$ such that the *finite double shuffle* (FDS) property holds:

$$Z_R(\omega_1 ш \omega_2) = Z_R(\omega_1 * \omega_2) = Z_R(\omega_1) Z_R(\omega_2).$$

We then extend Z_R to $Z_R^{ш}$ and Z_R^* as before. Define an R-module automorphism ρ_R of $R[T]$ by

$$\rho_R(e^{Tu}) = A_R(u) e^{Tu}$$

where

$$A_R(u) = \exp\left(\sum_{n=2}^{\infty} \frac{(-1)^n}{n} Z_R(a^{n-1}b_0) u^n \right) \in R[\![u]\!].$$

If a map $Z_R : \mathfrak{A}^0 \longrightarrow R$ satisfies the FDS and $(Z_R^{ш} - \rho_R \circ Z_R^*)(\omega) = 0$ for all $\omega \in \mathfrak{A}^1$ then we say that Z_R has the *regularized double shuffle* (RDS) property. Let R_{RDS} be the universal algebra (together with a map $Z_{RDS} : \mathfrak{A}^0 \longrightarrow R_{RDS}$) such that for every $\mathbb{Q}$-algebra R and a map $Z_R : \mathfrak{A}^0 \longrightarrow R$ satisfying RDS there always exists a map φ_R to make the following diagram commutative:

$$\begin{array}{ccc} \mathfrak{A}^0 & \xrightarrow{Z_{RDS}} & R_{RDS} \\ & \searrow^{Z_R} & \downarrow \varphi_R \\ & & R \end{array}$$

When $N = 2$ computation by Blümlein, Broadhurst and Vermaseren [5] shows that the finite distribution relations and the regularized distribution relations (18) contribute non-trivially when the weight $w = 8$ and $w = 11$, respectively. When $N = 3$ computation shows that the lifted relations contribute non-trivially when the weight $w = 4$ (see §5) and $w = 5$: we can only get $d(5, 3) \leq 33$ instead of the conjecturally correct dimension 32 without using the lifted relations. Note that in this case there are 612 FDS of weight five, 191 RDS of weight five, 8 FDT and 7 RDT.

One may use the fact that Z_R is an algebra homomorphism to produce *lifted finite double shuffle* and *lifted regularized double shuffle* relations as follows: for all $\omega_1 \in \mathfrak{A}^1$, $\omega_0, \omega_0', \omega_0'' \in \mathfrak{A}^0$ with $\lg(\omega_1) + \lg(\omega_0) = \lg(\omega_0) + \lg(\omega_0') + \lg(\omega_0'') = w$

$$Z_R^{ш}(\omega_1 ш \omega_0) - \rho_R \circ Z_R^*(\omega_1) Z_R^{ш}(\omega_0) = 0, \quad Z_R\big((\omega_0 * \omega_0') * \omega_0'' - (\omega_0 ш \omega_0') * \omega_0''\big) = 0.$$

In general, one can define the universal objects Z_{SR} and R_{SR} corresponding to the standard relations similar to Z_{RDS} and R_{RDS} such that for every $\mathbb{Q}$-algebra R and a map $Z_R : \mathfrak{A}^0 \longrightarrow R$ satisfying the standard relations there always exists a map φ_R to make the following diagram commutative:

$$\begin{array}{ccc} \mathfrak{A}^0 & \xrightarrow{Z_{SR}} & R_{SR} \\ & \searrow^{Z_R} & \downarrow \varphi_R \\ & & R \end{array} \qquad (20)$$

Recall that one has the evaluation map $Z : \mathfrak{A}^0 \longrightarrow \mathbb{C}$ by Prop. 2.8 which extends (5).

Conjecture 6.1. *Let* $(R, Z_R) = (\mathbb{R}, Z)$ *if* $N = 1$*, and* $(R, Z_R) = (\mathbb{C}, Z)$ *if* $N = 2, 3$ *or* $N = p^n$ *with prime* $p \geq 5$*. If* $N = 1$ *(resp.* $N = 2$*) then the map* $\varphi_{\mathbb{R}}$ *is injective, namely, the algebra of MPVs of level one or two is isomorphic to* R_{RDS} *(resp.* R_{SR}*). If* $N = 3$ *or* $N = p^n$ *(*$p \geq 5$*) then the map* $\varphi_{\mathbb{C}}$ *is injective so the algebra of MPVs of level* N *is isomorphic to* R_{SR}*.*

The above conjecture generalizes [24, Conjecture 1]. It means that all the linear relations among MPVs can be produced by RDS when $N = 1$ or 2, and by the standard ones when $N = 3$ or p^n with prime $p \geq 5$. When $N = p \geq 5$, p a prime, this is proved in Thm. 8.6 under the assumption of a variant of Grothendieck's period conjecture.

Computation in many cases such as those listed in Remark 8.2 and Conjecture 8.5 show that MPVs must satisfy some other relations apart from the standard ones when N has at least two distinct prime factors, so a naive generalization of Conjecture 6.1 to all levels does not exist at present. However, when $N = 4$ one can show that octahedral symmetry of $\mathbb{P}^1 - (\{0, \infty\} \cup \boldsymbol{\mu}_4)$ provide all the non-standard relations under the standard assumption (see Thm. 9.1). But since we only have numerical evidence in weight three and weight four it may be a little premature to form a conjecture for level four.

7 The structure of MPVs and some examples

In this section we concentrate on RDS between MPVs of small weights. Most of the computations in this section are carried out by MAPLE. We have checked the consistency of these relations with many known ones and verified our results numerically using GiNac [27] and EZ-face [9].

By considering all the admissible words we see easily that the number of distinct MPVs of weight $w \geq 2$ and level N is $N^2(N+1)^{w-2}$ and there are at most $N(N+1)^{w-2}$ RDS (but not FDS). If $w \geq 4$ then the number of FDS is given by

$$(N-1)N^2(N+1)^{w-3} + \Big(\Big[\frac{w}{2}\Big] - 1\Big)N^4(N+1)^{w-4} = \Big(N^2\Big[\frac{w}{2}\Big] - 1\Big)N^2(N+1)^{w-4}.$$

If $w = 2$ (resp. $w = 3$) then the number of FDS is $(N-1)^2$ (resp. $N^2(N-1)$). Therefore, it is not hard to see that the number of standard relations grow polynomially with the level N but exponentially with the weight w.

7.1 Weight one

From §3 we know that all relations in weight one follow from (11) and (12), and no RDS exists. The relations in weight one are crucial for higher level cases because they provide the weight one relations considered in §3. Moreover, easy computation by (11) and (12) shows that there is a hidden integral structure, namely, in each level there exists a $\mathbb{Q}$-basis consisting of MPVs such that every other MPV is a $\mathbb{Z}$-linear combination of the basis elements. This fact is proved by Conrad [13, Theorem 4.6]. Similar results should hold for higher weight cases and we hope to return to this in a future publication [14].

7.2 WEIGHT TWO

There are N^2 MPVs of weight two and level N:

$$L_N(1,1|i,j), \quad L_N(2|j), \qquad 1 \le i \le N-1, 0 \le j \le N-1.$$

For $1 \le i, j < N$ the FDS $Z^*(y_{1,i} * y_{1,j}) = Z^{\text{Ш}}(y_{1,i} \text{Ш} y_{1,j})$ yields

$$L_N(2|i+j) + L_N(1,1|i,j) + L_N(1,1|j,i) = L_N(1,1|i,j-i) + L_N(1,1|j,i-j). \tag{21}$$

Now from RDS $\rho(Z^*(y_{1,0} * y_{1,i})) = Z^{\text{Ш}}(y_{1,0} \text{Ш} y_{1,i})$ we get for $1 \le i < N$

$$L_N(1,1|i,0) + L_N(2|i) = L_N(1,1|i,-i). \tag{22}$$

The FDT in (14) yields: for every divisor d of N, and $1 \le a, b < d' := N/d$

$$L_N(2|ad) = d \sum_{j=0}^{d-1} L_N(2|a+jd'), \tag{23}$$

$$L_N(1,1|ad,bd) = \sum_{j,k=0}^{d-1} L_N(1,1|a+jd', b+kd'). \tag{24}$$

To derive the RDT we can compare the coefficients of $x_1 x_{\mu^{ad}}$ in (18) and use Prop. 4.3 to get: for every divisor d of N, and $1 \le a < d'$

$$\begin{aligned} L_N(1|ad) \sum_{j=1}^{d-1} L_N(1|jd') = & \sum_{j=1}^{d-1} \sum_{k=0}^{d-1} L_N(1,1|jd', a+kd') \\ & - \sum_{k=0}^{d-1} L_N(1,1|a+kd', -a-kd') - L_N(1,1|ad,-ad). \end{aligned} \tag{25}$$

By definition, the weight one relations are obtained from (11) and (12). For example, if $N = p$ is a prime then (12) is trivial and (11) is equivalent to the following: for all $1 \le j < h$ ($h := (p-1)/2$)

$$L_N(1|j) - L_N(1|-j) = (p-2j)(L_N(1|h) - L_N(1|h+1)). \tag{26}$$

Thus multiplying by $L_N(1|i)$ ($1 \le i < p$) and applying the shuffle relation $L_N(1|a)L_N(1|b) = L_N(1^2|a,b-a) + L_N(1^2|b,a-b)$ (here we put $L_N(1^2|-) = L_N(1,1|-)$ to save space) we get:

$$\begin{aligned} & L_N(1^2|i,j-i) + L_N(1^2|j,i-j) - L_N(1^2|i,-j-i) - L_N(1^2|-j,i+j) \\ = & (p-2j)\big(L_N(1^2|i,h-i) + L_N(1^2|h,i-h) - L_N(1^2|i,-i-h) - L_N(1^2|-h,i+h)\big). \end{aligned} \tag{27}$$

Computation shows that the following conjecture should hold.

Conjecture 7.1. *The RDT* (25) *follows from the combination of the following relations: the weight one relations, the RDS* (21) *and* (22)*, and the FDT* (23) *and* (24)*.*

7.3 Weight three

Apparently there are $N^2(N+1)$ MPVs of weight three and level N: for each choice (i,j,k) with $1 \le i \le N-1, 0 \le j,k \le N-1$ we have four MPVs of level N:

$$L_N(1^3|i,j,k) := L_N(1,1,1|i,j,k), \quad L_N(1,2|i,j), \quad L_N(2,1|j,k), \quad L_N(3|k).$$

For $1 \le i,j,k < N$ the FDS $Z^*\big(y_{1,i} * (y_{1,j}y_{1,k})\big) = Z^{Ш}\big(y_{1,i}Ш(y_{1,j}y_{1,k})\big)$ yields

$$\begin{aligned} L_N(1^3|i,j-i,k) &+ L_N(1^3|j,i-j,k+j-i) + L_N(1^3|j,k,i-k-j) \\ &= L_N(2,1|i+j,k) + L_N(1,2|j,i+k) \\ &\quad + L_N(1^3|i,j,k) + L_N(1^3|j,i,k) + L_N(1^3|j,k,i). \end{aligned} \tag{28}$$

For $1 \le i,j < N$ the FDS $Z^*(y_{1,i} * y_{2,j}) = Z^{Ш}(y_{1,i}Шy_{2,j})$ yields

$$\begin{aligned} L_N(3|i+j) &+ L_N(1,2|i,j) + L_N(2,1|j,i) \\ &= L_N(1,2|i,j-i) + L_N(2,1|i,j-i) + L_N(2,1|j,i-j). \end{aligned} \tag{29}$$

Moreover, there are three ways to produce RDS. Since $\rho(T) = T$ the first family of RDS come from $Z^*\big(y_{1,0} * (y_{1,i}y_{1,i+j})\big) = Z^{Ш}\big(y_{1,0}Ш(y_{1,i}y_{1,i+j})\big)$ for $1 \le i \le N-1, 0 \le j \le N-1$:

$$\begin{aligned} y_{1,0} * (y_{1,i}y_{1,i+j}) &= y_{1,0}y_{1,i}y_{1,i+j} + y_{1,i}\tau_i(y_{1,0} * y_{1,j}) + y_{2,i}y_{1,i+j} \\ =& y_{1,0}y_{1,i}y_{1,i+j} + y_{1,i}y_{1,i}y_{1,i+j} + y_{1,i}y_{1,i+j}y_{1,i+j} + y_{1,i}y_{2,i+j} + y_{2,i}y_{1,i+j} \end{aligned}$$

On the other hand,

$$y_{1,0}Шy_{1,i}y_{1,i+j} = y_{1,0}y_{1,i}y_{1,i+j} + y_{1,i}y_{1,0}y_{1,i+j} + y_{1,i}y_{1,i+j}y_{1,0}.$$

Hence

$$\begin{aligned} L_N(1^3|i,0,j) &+ L_N(1^3|i,j,0) + L_N(1,2|i,j) + L_N(2,1|i,j) \\ &= L_N(1^3|i,-i,i+j) + L_N(1^3|i,j,-i-j). \end{aligned} \tag{30}$$

The second family of RDS follow from $\rho(Z^*(y_{1,0} * y_{2,i})) = Z^{Ш}(y_{1,0}Шy_{2,i})$:

$$y_{1,0}y_{2,i} + y_{2,i}y_{1,i} + y_{3,i} = y_{1,0}y_{2,i} + y_{2,0}y_{1,i} + y_{2,i}y_{1,0}$$

which implies that

$$L_N(2,1,i,0)+L_N(3,i)=L_N(2,1,i,-i)+L_N(2,1,0,i). \quad (31)$$

Now we consider the last family of RDS. By the definition of stuffle product:

$$\begin{aligned} y_{1,0}*y_{1,0}*y_{1,i} =&(2y_{1,0}^2+y_{2,0})*y_{1,i}\\ =&2y_{1,0}(y_{1,0}*y_{1,i})+2y_{1,i}^3+2y_{2,i}y_{1,i}+y_{2,0}*y_{1,i}\\ =&2y_{1,0}^2y_{1,i}+2y_{1,0}y_{1,i}^2+2y_{1,0}y_{2,i}+2y_{1,i}^3+2y_{2,i}y_{1,i}+y_{2,0}*y_{1,i}. \end{aligned}$$

Applying $\rho\circ Z^*$ and noticing that $Z^{ш}_{(2|0)}(T)=\zeta(2)$ we get

$$\begin{aligned} (T^2+\zeta(2))Z^{ш}_{(1|i)}(T)=2Z^{ш}_{(1^3|0,0,i)}(T)+2Z^{ш}_{(1^3|0,i,i)}(T)+2Z^{ш}_{(1,2|0,i)}(T)\\ +2Z^{ш}_{(1^3|i,i,i)}(T)+2Z^{ш}_{(2,1|i,i)}(T)+Z^{ш}_{(2|0)}(T)Z^{ш}_{(1|i)}(T). \quad (32) \end{aligned}$$

On the other hand by the definition of shuffle product

$$y_{1,0}шy_{1,0}шy_{1,i}=2y_{1,0}^2шy_{1,i}=2y_{1,0}^2y_{1,i}+2y_{1,0}y_{1,i}y_{1,0}+2y_{1,i}y_{1,0}^2$$

Applying $Z^{ш}$ we get

$$T^2Z^{ш}_{(1|i)}(T)=2Z^{ш}_{(1^3|0,0,i)}(T)+2Z^{ш}_{(1^3|0,i,0)}(T)+2Z^{ш}_{(1^3|i,0,0)}(T). \quad (33)$$

We further have

$$\begin{aligned} &Z^{ш}(y_{1,0}y_{1,i}^2+y_{1,0}y_{2,i}-y_{1,0}y_{1,i}y_{1,0})\\ =&Z^{ш}(1^3|0,i,i)(T)+Z^{ш}_{(1,2|0,i)}(T)-Z^{ш}_{(1^3|0,i,0)}(T)\\ =&2Z^{ш}_{(1^3|i,0,0)}(T)-Z^{ш}_{(2,1|i,0)}(T)-Z^{ш}_{(2,1|0,i)}(T)-Z^{ш}_{(1^3|i,0,i)}(T)-Z^{ш}_{(1^3|i,i,0)}(T) \end{aligned}$$

where we have used the facts that

$$\begin{aligned} Z^{ш}_{(1,2|0,i)}(T)=&TZ^{ш}_{(2|i)}(T)-Z^{ш}_{(2,1|i,0)}(T)-Z^{ш}_{(2,1|0,i)}(T)\\ Z^{ш}_{(1^3|0,i,i)}(T)=&TZ^{ш}_{(1,1|i,i)}(T)-Z^{ш}_{(1^3|i,0,i)}(T)-Z^{ш}_{(1^3|i,i,0)}(T)\\ Z^{ш}_{(1^3|0,i,0)}(T)=&TZ^{ш}_{(1,1|i,0)}-2Z^{ш}_{(1^3|i,0,0)}(T)\\ Z^{ш}_{(1,1|i,0)}(T)=&Z^{ш}_{(2|i)}(T)+Z^{ш}_{(1,1|i,i)}(T). \end{aligned}$$

Hence for $1\le i<N$ we have by subtracting (33) from (32)

$$\begin{aligned} L_N(1^3|i,0,0)+L_N(2,1|i,0)+L_N(1^3|i,-i,0)=\\ L_N(2,1|i,-i)+L_N(2,1|0,i)+L_N(1^3|i,-i,i)+L_N(1^3|i,0,-i). \quad (34) \end{aligned}$$

Setting $j=0$ in (30) and subtracting from (34) we get

$$L_N(1^3|i,-i,0)=L_N(2,1|i,-i)+L_N(2,1|0,i)+L_N(1^3|i,0,0)+L_N(1,2|i,0). \quad (35)$$

7.4 Upper bound of $d(w, N)$ by Deligne and Goncharov

By using the theory of motivic fundamental groups of $\mathbb{P}^1 - (\{0, \infty\} \cup \boldsymbol{\mu}_N)$ Deligne and Goncharov [17, 5.25] show that $d(w, N) \le D(w, N)$ where $D(w, N)$ are defined by the formal power series

$$1 + \sum_{w=1}^{\infty} D(w, N) t^w = \begin{cases} (1 - t^2 - t^3)^{-1}, & \text{if } N = 1; \\ (1 - t - t^2)^{-1}, & \text{if } N = 2; \\ (1 - at + bt^2)^{-1}, & \text{if } N \ge 3, \end{cases} \tag{36}$$

where $a = a(N) := \varphi(N)/2 + \nu(N)$, $b = b(N) := \nu(N) - 1$, φ is the Euler's totient function and $\nu(N)$ is the number of distinct prime factors of N. If $N > 2$ then we have

$$\sum_{w=1}^{\infty} D(w, N) t^w = at + (a^2 - b)t^2 + (a^3 - 2ab)t^3 + (a^4 - 3a^2 b + b^2)t^4 + \cdots$$

In particular, if p is a prime then for any positive integer n

$$D(w, p^n) = a(p^n)^w = \left(\frac{p^{n-1}(p-1)}{2} + 1 \right)^w. \tag{37}$$

We will compare the bound obtained by the standard relations to the bound $D(w, N)$ in the next two sections.

8 Computational results in weight two

In this section we combine the analysis in the previous sections and the theory developed by Deligne and Goncharov [17] to present a detailed computation in weight two and level $N \le 169$.
Let $\mathcal{G} := \iota(\mathrm{Lie}\, U_\omega)$ be the motivic fundamental Lie algebra (see [17, (5.12.2)]) associated to the motivic fundamental group of $\mathbb{P}^1 - (\{0, \infty\} \cup \boldsymbol{\mu}_N)$. As pointed out in §6.13 of op. cit. one may safely replace $\mathcal{G}(\boldsymbol{\mu}_N)^{(\ell)}$ by $\mathcal{G}$ throughout [20]. Then it follows from the proof of [17, 5.25] that if conjecture [17, 5.27(c)] is true, which we assume in the following, then

$$d(2, N) = D(2, N) - \dim \ker(\beta_N), \tag{38}$$

where $\beta_N : \bigwedge^2 \mathcal{G}_{-1,-1} \longrightarrow \mathcal{G}_{-2,-2}$ is given by Ihara's bracket $\beta_N(a \wedge b) = \{a, b\}$ defined by (5.13.6) of op. cit. Here $\mathcal{G}_{\bullet,\bullet}$ is the associated graded of the weight and depth gradings of $\mathcal{G}$ (see [20, §2.1]). Let $k(N) := \dim \ker(\beta_N)$. Then

$$\delta_1(N) := \dim \mathcal{G}_{-1,-1} = \begin{cases} 1, & \text{if } N = 1 \text{ or } 2; \\ \varphi(N)/2 + \nu(N) - 1, & \text{if } N \ge 3, \end{cases} \tag{39}$$

by [20, Thm. 2.1]. Thus

$$i(N) := \dim \mathrm{Im}(\beta_N) = \delta_1(N)(\delta_1(N) - 1)/2 - k(N). \tag{40}$$

N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
δ_1	1	1	1	1	2	2	3	2	3	3	5	3	6	4	5	4
i	0	0	0	0	0	1	1	1	3	3	5	3	8	6	10	6
k	0	0	0	0	1	0	2	0	0	0	5	0	7	0	0	0
δ_2	0	0	1	1	2	2	4	3	6	5	10	5	14	9	14	10
sr	0	0	1	1	2	2	4	4	6	6	10	8	14	12	16	16
D	1	2	4	4	9	8	16	9	16	15	36	15	49	24	35	25
SR	1	2	4	4	8	8	14	10	16	16	31	18	42	27	37	31
d	1	2	4	4	8	8	14	9	16	15	31	15	42	24	35	25

N	17	18	19	20	21	22	23	24	25	26	27	28	29
δ_1	8	4	9	5	7	6	11	5	10	7	9	7	14
i	16	6	21	10	21	15	33	10	40	21	36	21	56
k	12	0	15	0	0	0	22	0	5	0	0	0	35
δ_2	24	9	30	14	27	20	44	14	50	27	45	27	70
sr	24	18	30	24	32	30	44	32	50	42	54	48	70
D	81	24	100	35	63	48	144	35	121	63	100	63	225
SR	69	33	85	45	68	58	122	53	116	78	109	84	190
d	69	24	85	35	63	48	122	35	116	63	100	63	190

N	30	31	32	33	34	35	36	37	38	39	40	41
δ_1	6	15	8	11	9	13	7	18	10	13	9	20
i	15	65	28	55	36	78	21	96	45	78	36	120
k	0	40	0	0	0	0	0	57	0	0	0	70
δ_2	19	80	36	65	44	90	27	114	54	90	44	140
sr	48	80	64	80	72	96	72	114	90	112	96	140
D	47	256	81	143	99	195	63	361	120	195	99	441
SR	76	216	109	158	127	201	108	304	156	217	151	371
d	47	216	81	143	99	195	63	304	120	195	99	371

N	42	43	44	45	46	47	48	49	121	125	169
δ_1	8	21	11	13	12	23	9	21	55	50	78
i	28	133	55	78	66	161	36	175	1155	1200	2288
k	0	77	0	0	0	92	0	35	330	25	715
δ_2	34	154	65	90	77	184	44	196	1210	1250	2366
sr	96	154	120	144	132	184	128	196	1210	1250	2366
D	79	484	143	195	168	576	99	484	3136	2601	6241
SR	141	407	198	249	223	484	183	449	2806	2576	5526
d	79	407	143	195	168	484	99	449	2806	2576	5526

Table 1: Upper bounds of $d(2, N)$ by the standard relations and [17, 5.25].

Since $\dim \mathcal{G}_{-2,-1} = \varphi(N)/2$ if $N > 2$ and 0 otherwise the dimension of the degree two part of $\mathcal{G}$ is

$$\delta_2(N) := \dim \mathcal{G}_{-2,-1} + \dim \mathcal{G}_{-2,-2} = \begin{cases} i(N), & \text{if } N = 1 \text{ or } 2; \\ \varphi(N)/2 + i(N), & \text{if } N \geq 3. \end{cases} \tag{41}$$

Let $sr(N)$ be the upper bound of $\delta_2(N)$ obtained by the standard relations. This can be computed by the method described in [30, §2]. Let $SR(N)$ be the upper bound of $d(2, N)$ similarly obtained by the standard relations. In Table 1 we use MAPLE to provide the following data: $k(N)$, $sr(N)$, and $SR(N)$. Then we can calculate $\delta_1(N)$, $i(N)$ and $\delta_2(N)$ by (39), (40) (41), respectively. From (38) we can check the consistency by verifying

$$sr(N) - \delta_2(N) = SR(N) - d(2, N) = SR(N) - D(2, N) + k(N)$$

which gives the number of linearly independent non-standard relations (assuming the conjecture in [17, 5.27(c)]). In Table 1 we provide some computational data of the above quantities. To save space we write $D = D(2, N)$ and $d = d(2, N)$.

Definition 8.1. We call the level N *standard* if either (i) $N = 1, 2$ or 3, or (ii) N is a prime power p^n ($p \geq 5$). Otherwise N is called *non-standard*.

Remark 8.2. We now make the following comments in the weight two case from Table 1.
(a) When $p \geq 11$ the vector space $\ker \beta_p$ contains a subspace isomorphic to the space of cusp forms of weight two on $X_1(p)$ which has dimension $(p-5)(p-7)/24$ (see [20, Lemma 2.3 & Theorem 7.8]). So it must contain another piece which has dimension $(p-3)/2$ since $\dim(\ker \beta_p) = (p^2 - 1)/24$ by [30, (6)]. One may wonder if this missing piece has any significance in geometry and/or number theory.
(b) If N is a 2-power or a 3-power then $D(2, N)$ should be sharp. See Remark 5.4.
(c) If N has at least two distinct prime factors then $D(2, N)$ seems to be sharp, though we don't have any theory to support it.
(d) Suppose the conjecture in [17, 5.27(c)] is true. Then by [17, 5.27], (b) and (c) is equivalent to saying that the kernel of β_N is trivial if the level N is non-standard. We believe this is also a necessary condition on N for β_N to be trivial.
(e) If the level $N > 3$ is standard then β_N is *unlikely* to be injective. We conjecture that non-standard relation doesn't exist (i.e., $SR(N)$ is sharp), though for prime power levels we only have verified this for the first four prime square levels $N = 5^2, 7^2, 11^2, 13^2$, and the first cubic power level $N = 5^3$.

The equation $\dim \beta_p = (p^2 - 1)/24$ (see [30, (6)]) together with Theorem 8.6 confirms Remark 8.2(e) for prime levels if we assume a variant of Grothendieck's period conjecture [17, 5.27(c)]. The next result partially confirms Remark 8.2(e) in the case when the level is a prime square.

THEOREM 8.3. *If* $p \geq 5$ *is a prime then* $\ker \beta_{p^2} \neq 0$ *and*

$$d(2,p^2) < D(2,p^2) = (p^2 - p + 2)^2/4.$$

Proof. By the proof of Delign-Goncharov's bound $D(2,p^2)$ in [17, 5.25] we only need to show $\ker \beta_{p^2} \neq 0$. In the following we adopt the same notation as in [17] and [30].

Fix a primitive p^2th root of unity μ. Put $e(a) = e_{\mu^a}$ for all integer a. Define

$$g_{k,j} = e(pk + j) + e(p^2 - pk - j) + e(pj) + e(p^2 - pj)$$

for $0 \leq k < (p-1)/2$, $1 \leq j \leq p-1$, and for $k = (p-1)/2$, $1 \leq j \leq (p-1)/2$. One only needs to prove the following

CLAIM. Let $h = (p-3)/2$. Then one has

$$\sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} + \sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1}, g_{h+1,j}\}$$
$$+\sum_{k=0}^{h}\sum_{l=k+1}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1}, g_{l,j}\} + \sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1}, g_{h+1,j}\}$$
$$-\sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,j}, g_{l,p-1}\} - \sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,j}, g_{l+1,1}\} = 0.$$

There are $h(2h+3)^2 = hp^2$ distinct terms on the left, each with coefficient ± 1.

The proof of the claim is straight-forward by a little tedious change of indices and regrouping.

$$-\sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,j}, g_{l+1,1}\} = \sum_{k=0}^{h}\sum_{l=0}^{k}\sum_{j=2}^{p-2}\{g_{k+1,1}, g_{l,j}\} = \sum_{k=1}^{h+1}\sum_{l=0}^{k-1}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\}.$$

Then the expression in the claim becomes

$$\sum_{k=1}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} + \sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{0,1}, g_{l,j}\} + \sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{h+1,1}, g_{l,j}\}$$
$$+\sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1}, g_{h+1,j}\} + \sum_{k=0}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1}, g_{l,j}\} + \sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1}, g_{h+1,j}\}$$
$$= \sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} + \sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1}, g_{h+1,j}\}$$
$$+\sum_{k=0}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1}, g_{l,j}\} + \sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1}, g_{h+1,j}\}.$$

Let us write $\{a,b\} = \{e(a), e(b)\}$. By definition

$$
\begin{aligned}
&\{g_{k,1}, g_{l,j}\}\\
=&\{pk+1, pl+j\} + \{-pk-1, pl+j\} + \{p, pl+j\} + \{-p, pl+j\}\\
+&\{pk+1, -pl-j\} + \{-pk-1, -pl-j\} + \{p, -pl-j\} + \{-p, -pl-j\}\\
+&\{pk+1, pj\} + \{-pk-1, pj\} + \{p, pj\} + \{-p, pj\}\\
+&\{pk+1, -pj\} + \{-pk-1, -pj\} + \{p, -pj\} + \{-p, -pj\}\\
=&\{pk+1, pl+j\} + \{p(p-k)-1, pl+j\} + \{p, pl+j\} + \{-p, pl+j\}\\
+&\{pk+1, p(p-1-l)+p-j\} + \{p(p-k)-1, p(p-1-l)+p-j\}\\
&\qquad + \{p, p(p-1-l)+p-j\} + \{-p, p(p-1-l)+p-j\}\\
+&\{pk+1, pj\} + \{p(p-k)-1, pj\} + \{p, pj\} + \{-p, pj\}\\
+&\{pk+1, p(p-j)\} + \{p(p-k)-1, p(p-j)\} + \{p, p(p-j)\} + \{-p, p(p-j)\}.
\end{aligned}
$$

Then

$$
\begin{aligned}
&\sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} = \sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{pk+1, pl+j\} + \{p(p-k)-1, pl+j\}\\
+&\{pk+1, p(p-1-l)+j\} + \{p(p-k)-1, p(p-1-l)+j\}\\
+&\{p, pl+j\} + \{-p, pl+j\} + \{p, p(p-1-l)+j\} + \{-p, p(p-1-l)+j\}\\
+&2\{pk+1, pj\} + 2\{p(p-k)-1, pj\} + 2\{p, pj\} + 2\{-p, pj\}\\
=&\sum_{k=0}^{h+1}\sum_{l=0, l\neq h+1}^{p-1}\sum_{j=2}^{p-2}\{pk+1, pl+j\} + \sum_{k=h+2}^{p}\sum_{l=0, l\neq h+1}^{p-1}\sum_{j=2}^{p-2}\{pk-1, pl+j\}\\
+&\sum_{k=0}^{h+1}\sum_{l=0, l\neq h+1}^{p-1}\sum_{j=2}^{p-2}\Big(\{p, pl+j\} + \{-p, pl+j\}\Big) + 2(h+1)\sum_{k=0}^{h+1}\sum_{j=2}^{p-2}\{pk+1, pj\}\\
+&2(h+1)\sum_{k=h+2}^{p}\sum_{j=2}^{p-2}\{pk-1, pj\} + 2(h+2)(h+1)\sum_{j=2}^{p-2}\Big(\{p, pj\} + \{-p, pj\}\Big).
\end{aligned}
$$

Thus

$$
\begin{aligned}
&\sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} + \sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1}, g_{h+1,j}\}\\
=&\sum_{k=0}^{h+1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1, pl+j\} + \sum_{k=h+2}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk-1, pl+j\}\\
+&\frac{p+1}{2}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big(\{p, pl+j\} + \{-p, pl+j\}\Big) + p\sum_{k=0}^{h+1}\sum_{j=2}^{p-2}\{pk+1, pj\}\\
+&p\sum_{k=h+2}^{p}\sum_{j=2}^{p-2}\{pk-1, pj\} + \frac{p(p+1)}{2}\sum_{j=2}^{p-2}\Big(\{p, pj\} + \{-p, pj\}\Big).
\end{aligned}
$$

Similarly,

$$\begin{aligned}
&\sum_{k=0}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1},g_{l,j}\}+\sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1},g_{h+1,j}\}\\
=&\sum_{k=1}^{h+1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk-1,pl+j\}+\sum_{k=h+2}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pl+j\}\\
+&\frac{p-1}{2}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big(\{p,pl+j\}+\{-p,pl+j\}\Big)+p\sum_{k=1}^{h+1}\sum_{j=2}^{p-2}\{pk-1,pj\}\\
+&p\sum_{k=h+2}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pj\}+\frac{p(p-1)}{2}\sum_{j=2}^{p-2}\Big(\{p,pj\}+\{-p,pj\}\Big).
\end{aligned}$$

Altogether the expression in the claim is reduced to

$$\begin{aligned}
X:=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pl+j\}+\sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk-1,pl+j\}\\
&+p\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big(\{p,pl+j\}+\{-p,pl+j\}\Big)+p\sum_{k=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pj\}\\
&+p\sum_{k=1}^{p}\sum_{j=2}^{p-2}\{pk-1,pj\}+p^2\sum_{j=2}^{p-2}\Big(\{p,pj\}+\{-p,pj\}\Big).
\end{aligned}$$

To see this last expression can be reduced to 0 we recall that by definition [17, (5.13.6)]

$$\{a,b\}=\{e_a,e_b\}=[e_a,e_b]+\partial_a(e_b)-\partial_b(e_a),$$

where ∂_a is the derivation defined by $\partial_a(e_0)=0$ and $\partial_a(e_\zeta)=[-[\zeta](e_a),e_\zeta]$ for any p^2th root of unity ζ (see [17, (5.13.4)]). Thus by abuse of notation $[x,y]=[e(x),e(y)]$ we get

$$\begin{aligned}
X=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big([pk+1,pl+j]-[p(k+l)+j+1,pl+j]\\
&\qquad\qquad+[p(k+l)+j+1,pk+1]\Big) \qquad (42)\\
&+\sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big([pk-1,pl+j]-[p(k+l)+j-1,pl+j]\\
&\qquad\qquad+[p(k+l)+j-1,pk-1]\Big) \qquad (43)\\
&+p\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big([p,pl+j]-[p(l+1)+j,pl+j]+[p(l+1)+j,p]
\end{aligned}$$

$$+[-p, pl+j] - [p(l-1)+j, pl+j] + [p(l-1)+j, -p]\Big) \tag{44}$$

$$+p\sum_{k=0}^{p-1}\sum_{j=2}^{p-2}\Big([pk+1, pj] - [p(j+k)+1, pj] + [p(j+k)+1, pk+1]\Big) \tag{45}$$

$$+p\sum_{k=1}^{p}\sum_{j=2}^{p-2}\Big([pk-1, pj] - [p(j+k)-1, pj] + [p(j+k)-1, pk-1]\Big) \tag{46}$$

$$+p^2\sum_{j=2}^{p-2}\Big([p, pj] - [p(j+1), pj] + [p(j+1), p] + [-p, pj] - [p(j-1), pj] + [p(j-1), -p]\Big). \tag{47}$$

Now by skew-symmetry of Lie bracket

$$\begin{aligned}
&(42)+(43)\\
=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}[pk+1, pl+j] + \sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}[pk+j, pl+j+1]\\
-&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=3}^{p-1}[pk+1, pl+j] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}[pk-1, pl+j]\\
-&\sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=1}^{p-3}[p(k+l)+j, pl+j+1] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=1}^{p-3}[pl+j, pk-1]\\
=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}[pk+1, pl+2] + \sum_{k=0}^{p-1}\sum_{l=0}^{p-1}[pk+p-2, pl+p-1]\\
-&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}[pk+1, pl+p-1] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}[pk-1, pl+p-2]\\
-&\sum_{k=1}^{p}\sum_{l=0}^{p-1}[pk+1, pl+2] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}[pl+1, pk-1] = 0.
\end{aligned}$$

Similarly we can easily find that (44) = (45) = (46) = (47) = 0. This finishes the proof of the theorem. □

Remark 8.4. The theorem corrects a misprint in the statement of [30, Thm. 2].

In the three cases $(w, N) = (2, 8), (2, 10)$ and $(2, 12)$ we see that $SR(N) > d(w; N) = D(w; N)$. By numerical computation we have

Conjecture 8.5. *We have*

$$d(2, 8) = 9, \quad d(2, 10) = d(2, 12) = 15,$$

and the following relations are the linearly independent non-standard relations: let $L_N(-) = L_N(1,1|-)$ *and* $L_N^{(2)}(-) = L_N(2|-)$*, then*

$$\begin{aligned}
37L_8(1,1) =&34L_8^{(2)}(5) + 112L_8(3,1) + 11L_8(3,0) + 37L_8^{(2)}(1) - 2L_8(2,6)\\
&+ 3L_8(7,3) - 111L_8(5,7) + 38L_8(7,7) - 8L_8(5,5), \qquad (48)\\
7L_{10}(5,2) =&72L_{10}^{(2)}(1) + 265L_{10}^{(2)}(7) - 7L_{10}(2,5) + 64L_{10}(9,8) + 14L_{10}(5,6)\\
&- 467L_{10}(4,2) + 467L_{10}(8,6) - 164L_{10}(9,4) + 166L_{10}(7,9)\\
&- 260L_{10}(8,1) - 66L_{10}(3,9) - 7L_{10}(6,9) + 7L_{10}(6,5). \qquad (49)\\
L_{12}(8,7) =&5L_{12}^{(2)}(5) + 8L_{12}(8,10) - 6L_{12}(10,11) - 8L_{12}(9,11) + L_{12}(10,9)\\
&- 15L_{12}(8,1) + 5L_{12}(9,10) + 5L_{12}(6,1) - L_{12}(1,1)\\
&+ 6L_{12}(8,11) - 11L_{12}(6,11) + 8L_{12}(8,3) - L_{12}(11,8), \qquad (50)\\
60L_{12}(8,11) =&38L_{12}(8,7) + 348L_{12}(10,11) + 502L_{12}(9,11)\\
&- 492L_{12}(10,9) + 600L_{12}(8,1) - 552L_{12}(9,10)\\
&- 154L_{12}(11,10) + 20L_{12}(6,1) + 261L_{12}(6,11)\\
&- 502L_{12}(8,3) + 221L_{12}(11,8) - 319L_{12}(8,10), \qquad (51)\\
221L_{12}(1,1) =&1854L_{12}(8,10) + 562L_{12}(8,7) - 1018L_{12}(10,11)\\
&- 2416L_{12}(9,11) + 319L_{12}(10,9) - 4270L_{12}(8,1)\\
&+ 2293L_{12}(9,10) + 956L_{12}(11,10) + 1110L_{12}(6,1)\\
&+ 2416L_{12}(8,11) - 3305L_{12}(6,11) + 2416L_{12}(8,3). \qquad (52)
\end{aligned}$$

When N is a non-standard level we find that very often there are non-standard relations among MPVs. For examples, the five relations in Conjecture 8.5 are discovered only through numerical computation. On the other hand, we expect that the standard relations are enough to produce all the linear relations when N *is* standard. In weight two, when N is a prime the answer is confirmed by the next theorem if one assumes a variant of Grothendieck's period conjecture. Computations above provided the primary motivation of this result at the initial stage of this work.

THEOREM 8.6. ([30]) *Let* $p \geq 5$ *be a prime. Then*

$$d(2,p) \leq \frac{(5p+7)(p+1)}{24}.$$

If the conjecture in [17, 5.27(c)] *is true then the equality holds and the standard relations in* $\mathcal{MPV}(2,p)$ *imply all the others.*

Proof. See the proof of [30, Thm. 1]. □

It follows from [30, (6)] that the kernel β_p has dimension

$$k(p) = \frac{p^2-1}{24}$$

for all prime $p \geq 5$. From the data in Table 1 we have

Conjecture 8.7. *(a) For all prime $p \geq 5$ kernel β_{p^2} has dimension*

$$k(p^2) = \frac{p(p-1)(p-2)(p-3)}{24}.$$

As a consequence, the upper bound of $d(2,p^2)$ produced by the standard relations is

$$d(2,p^2) \leq \frac{5p^4 - 6p^3 + 19p^2 - 18p + 24}{24}.$$

(b) The standard relations produce all the linear relations and the upper bound in (a) is sharp.

Conjecture 8.8. *(a) For all prime $p \geq 5$ kernel β_{p^3} has dimension*

$$k(p^3) = \frac{p^2(p-1)(p-2)(p-3)(p-4)}{24}.$$

As a consequence, the upper bound of $d(2,p^3)$ produced by the standard relations is

$$d(2,p^3) \leq \frac{5p^6 - 2p^5 - 29p^4 + 74p^3 - 48p^2 + 24}{24}.$$

(b) The standard relations produce all the linear relations and the upper bound in (a) is sharp.

9 Computational results in weight three, four and five

In this last section we briefly discuss our results in weight three, four and five. Since the computational complexity increases exponentially with the weight we cannot do as many cases as we have done in weight two.

Combining the FDS (28), (29), RDS (30)-(35), and the weight one relations (13) and using MAPLE we have verified that $d(3,1) = 1, d(3,2) \leq 3, d(3,3) \leq 8$....

N	1	2	3	4	5	6	7
$SR(3)$	1	3	8	9	22	23	50
$D(3)$	1	3	8	8	27	21	64
$SR(4)$	1	5	16	21	61	69	
$D(4)$	1	5	16	16	81	55	256
$SR(5)$	2	8	32				
$D(5)$	2	8	32	32	243	144	1024
N	8	9	10	11	12	13	
$SR(3)$	38	67	70	157	94	246	
$D(3)$	27	64	56	216	56	343	

Table 2: Upper bounds of $d(w,N)$ by the standard relations and [17, 5.25].

We have done similar computation in other small weight and low level cases and listed the results in Table 2. The values of Deligne and Goncharov's bound $D(w) = D(w,N)$ in Table 2 should be compared with the bound $SR(w) = SR(w,N)$ obtained by the standard relations.
Note that $SR(3,4) = D(3,4)+1$. By numerical computation using EZface [9] and GiNac [27] we find the following non-standard relation in weight 3:

$$\begin{aligned}5L_4(1,2|2,3) =&46L_4(1,1,1|1,0,0) - 7L_4(1,1,1|2,2,1) - 13L_4(1,1,1|1,1,1)\\&+13L_4(1,2|3,1) - L_4(1,1,1|3,2,0) + 25L_4(1,1,1|3,0,0)\\&-8L_4(1,1,1|1,1,2) + 18L_4(2,1|3,0),\end{aligned} \tag{53}$$

and five non-standard relations in weight 4:

$$\begin{aligned}0 =&-255608l_1 - 265360l_2 - 219216l_3 - 19306179l_4 - 214008l_5 + 45560l_6\\&-148296l_7 - 1117280l_8 - 677152l_9 + 86512l_{10} - 239320l_{11} - 50032l_{12}\\&-121008l_{13} - 96944l_{14} + 202328l_{15} - 1178499l_{16} + 98944l_{17}\\&+1565754l_{18} + 23071580l_{19} + 363568l_{20} - 3310177l_{21},\end{aligned} \tag{54}$$

$$\begin{aligned}0 =&29752l_1 + 23312l_2 + 10960l_3 + 6123413l_4 + 16440l_5 - 12408l_6\\&+7144l_7 + 58272l_8 + 86976l_9 - 15952l_{10} + 41144l_{11} + 13552l_{12}\\&+29552l_{13} + 9840l_{14} - 36696l_{15} + 375805l_{16} - 41760l_{17}\\&-477366l_{18} - 7196900l_{19} - 62128l_{20} + 1048983l_{21},\end{aligned} \tag{55}$$

$$\begin{aligned}0 =&477444l_1 + 431352l_2 + 268168l_3 + 98404710l_4 + 308964l_5 - 233140l_6\\&+130028l_7 + 1563872l_8 + 1516032l_9 - 296664l_{10} + 702308l_{11} + 190136l_{12}\\&+506440l_{13} + 141592l_{14} - 636468l_{15} + 6027441l_{16} - 701600l_{17}\\&-7683609l_{18} - 115803282l_{19} - 1063768l_{20} + 16877562l_{21},\end{aligned} \tag{56}$$

$$\begin{aligned}0 =&-5976l_1 + 1776l_2 + 8496l_3 - 2132671l_4 + 3176l_5 + 1752l_6\\&+3832l_7 + 50976l_8 - 2688l_9 + 2320l_{10} - 10264l_{11} - 5808l_{12}\\&-6128l_{13} + 2320l_{14} + 8120l_{15} - 132307l_{16} + 13856l_{17}\\&+162614l_{18} + 2487604l_{19} + 12720l_{20} - 368485l_{21},\end{aligned} \tag{57}$$

$$\begin{aligned}0 =&-474064l_1 - 405248l_2 - 243520l_3 - 54556373l_4 - 283952l_5 + 84368l_6\\&-170640l_7 - 1033056l_8 - 994784l_9 + 174880l_{10} - 540432l_{11} - 156544l_{12}\\&-240512l_{13} - 49344l_{14} + 411152l_{15} - 3357683l_{16} + 292256l_{17}\\&+4291792l_{18} + 64572648l_{19} + 743136l_{20} - 9470695l_{21}.\end{aligned} \tag{58}$$

where by setting $L = L_4$, $1^4 = \{1\}^4$, ...

$$\begin{array}{lll}l_1 = L(1^4|2,1,0,1), & l_2 = L(1^4|2,1^2,0), & l_3 = L(1^4|2,0,3,1),\\ l_4 = L(1^4|2,0^3), & l_5 = L(1^4|1,2,0,3), & l_6 = L(1^4|3^2,0,3),\\ l_7 = L(1^4|3,1,3,2), & l_8 = L(1^4|3,0^3), & l_9 = L(1^4|3,0,1,0),\\ l_{10} = L(1^4|3,0,1^2), & l_{11} = L(2,1^2|0,3,0), & l_{12} = L(3,1|0,3),\\ l_{13} = L(1^4|2,2,3,0), & l_{14} = L(2,1^2|3,1^2), & l_{15} = L(2,1^2|3,0,3),\\ l_{16} = L(1^2,2|2^3), & l_{17} = L(1^4|2,0,1,0), & l_{18} = L(2,1^2|2^2,0),\\ l_{19} = L(1^4|\{2,0\}^2), & l_{20} = L(2^2|3,0), & l_{21} = L(1^4|2^4).\end{array}$$

We now can prove this by using the octahedral symmetry of $\mathbb{P}^1 - (\{0,\infty\} \cup \boldsymbol{\mu}_4)$ (see Remark 5.3). This idea was suggested to the author by Deligne in a letter dated Feb. 14, 2008.

Theorem 9.1. ([30]) *If the conjecture in* [17, 5.27(c)] *is true then all the linear relations among MPVs of level four and weight three (resp. weight four) are the consequences of the standard relations and the octahedral relation* (53) *(resp. the five octahedral relations* (54)-(58)*).*

Proof. For the proof please see[30, §3]. □

From the available data in Table 2 we can formulate the following conjecture.

Conjecture 9.2. *Suppose the level $N = p$ is a prime ≥ 5. Then*

$$d(3,p) \le \frac{p^3 + 4p^2 + 5p + 14}{12}.$$

Moreover, equality holds if standard relations produce all the linear relations.

We formulated this conjecture under the belief that the upper bound of $d(3,p)$ produced by the standard relations should be a polynomial of p of degree 3. Then we find the coefficients by the bounds of $d(3,p)$ for $p = 5, 7, 11, 13$ in Table 2.
When $w > 2$ it's not too hard to improve the bound of $d(w,p)$ given in [17, 5.25] by the same idea as used in the proof of [17, 5.24] (for example, decrease the bound by $(p^2 - 1)/24$). But they are often not the best. We conclude our paper with the following conjecture.

Conjecture 9.3. *If N is a standard level then the standard relations always provide the sharp bounds of $d(w,N)$, namely, all linear relations can be derived from the standard ones, if further $N > 3$ then the bound $D(w,N)$ in* (36) *by Deligne and Goncharov can be lowered. If N is a non-standard level then the bound $D(w,N)$ is sharp and there exists a positive integer $w_0(N)$ so that at least one non-standard relation exists in $\mathcal{MPV}(w,N)$ for each $w \ge w_0(N)$.*

It is likely that one can take $w_0(4) = w_0(6) = w_0(9) = 3$ and $w_0(N) = 2$ for all the other non-standard levels N.

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The Line Bundles on Moduli Stacks of Principal Bundles on a Curve

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Abstract. Let G be an affine reductive algebraic group over an algebraically closed field k. We determine the Picard group of the moduli stacks of principal G–bundles on any smooth projective curve over k.

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1. Introduction

As long as moduli spaces of bundles on a smooth projective algebraic curve C have been studied, their Picard groups have attracted some interest. The first case was the coarse moduli scheme of semistable vector bundles with fixed determinant over a curve C of genus $g_C \geq 2$. Seshadri proved that its Picard group is infinite cyclic in the coprime case [28]; Drézet and Narasimhan showed that this remains valid in the non–coprime case also [9].
The case of principal G–bundles over C for simply connected, almost simple groups G over the complex numbers has been studied intensively, motivated also by the relation to conformal field theory and the Verlinde formula [1, 12, 20]. Here Kumar and Narasimhan [19] showed that the Picard group of the coarse moduli scheme of semistable G–principal bundles over a curve C of genus $g_C \geq 2$ embeds as a subgroup of finite index into the Picard group of the affine Grassmannian, which is canonically isomorphic to $\mathbb{Z}$; this finite index was determined recently in [6]. Concerning the Picard group of the moduli stack $\mathcal{M}_G$ of principal G–bundles over a curve C of any genus $g_C \geq 0$, Laszlo and Sorger [23, 30] showed that its canonical map to the Picard group $\mathbb{Z}$ of the affine Grassmannian is actually an isomorphism. Faltings [13] has generalised this result to positive characteristic, and in fact to arbitrary noetherian base scheme.

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If G is not simply connected, then the moduli stack $\mathcal{M}_G$ has several connected components which are indexed by $\pi_1(G)$. For any $d \in \pi_1(G)$, let $\mathcal{M}_G^d$ be the corresponding connected component of $\mathcal{M}_G$. For semisimple, almost simple groups G over $\mathbb{C}$, the Picard group $\mathrm{Pic}(\mathcal{M}_G^d)$ has been determined case by case by Beauville, Laszlo and Sorger [2, 22]. It is finitely generated, and its torsion part is a direct sum of $2g_C$ copies of $\pi_1(G)$. Furthermore, its torsion–free part again embeds as a subgroup of finite index into the Picard group $\mathbb{Z}$ of the affine Grassmannian. Together with a general expression for this index, Teleman [31] also proved these statements, using topological and analytic methods.
In this paper, we determine the Picard group $\mathrm{Pic}(\mathcal{M}_G^d)$ for any reductive group G, working over an algebraically closed ground field k without any restriction on the characteristic of k (for all $g_C \geq 0$). Endowing this group with a natural scheme structure, we prove that the resulting group scheme $\underline{\mathrm{Pic}}(\mathcal{M}_G^d)$ over k contains, as an open subgroup, the scheme of homomorphisms from $\pi_1(G)$ to the Jacobian J_C, with the quotient being a finitely generated free abelian group which we denote by $\mathrm{NS}(\mathcal{M}_G^d)$ and call it the Néron–Severi group (see Theorem 5.3.1). We introduce this Néron–Severi group combinatorially in § 5.2; in particular, Proposition 5.2.11 describes it as follows: the group $\mathrm{NS}(\mathcal{M}_G^d)$ contains a subgroup $\mathrm{NS}(\mathcal{M}_{G^{\mathrm{ab}}})$ which depends only on the torus $G^{\mathrm{ab}} = G/[G, G]$; the quotient is a group of Weyl–invariant symmetric bilinear forms on the root system of the semisimple part $[G, G]$, subject to certain integrality conditions that generalise Teleman's result in [31].
We also describe the maps of Picard groups induced by group homomorphisms $G \longrightarrow H$. An interesting effect appears for the inclusion $\iota_G : T_G \hookrightarrow G$ of a maximal torus, say for semisimple G: Here the induced map $\mathrm{NS}(\mathcal{M}_G^d) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_G}^\delta)$ for a lift $\delta \in \pi_1(T_G)$ of d involves contracting each bilinear form in $\mathrm{NS}(\mathcal{M}_G^d)$ to a linear form by means of δ (cf. Definition 4.3.5). In general, the map of Picard groups induced by a group homomorphism $G \longrightarrow H$ is a combination of this effect and of more straightforward induced maps (cf. Definition 5.2.7 and Theorem 5.3.1.iv). In particular, these induced maps are different on different components of $\mathcal{M}_G$, whereas the Picard groups $\mathrm{Pic}(\mathcal{M}_G^d)$ themselves are essentially independent of d.
Our proof is based on Faltings' result in the simply connected case. To deduce the general case, the strategy of [2] and [22] is followed, meaning we "cover" the moduli stack $\mathcal{M}_G^d$ by a moduli stack of "twisted" bundles as in [2] under the universal cover of G, more precisely under an appropriate torus times the universal cover of the semisimple part $[G, G]$. To this "covering", we apply Laszlo's [22] method of descent for torsors under a group stack. To understand the relevant descent data, it turns out that we may restrict to the maximal torus T_G in G, roughly speaking because the pullback ι_G^* is injective on the Picard groups of the moduli stacks.
We briefly describe the structure of this paper. In Section 2, we recall the relevant moduli stacks and collect some basic facts. Section 3 deals with the case that $G = T$ is a torus. Section 4 treats the "twisted" simply connected case as indicated above. In the final Section 5, we put everything together to

prove our main theorem, namely Theorem 5.3.1. Each section begins with a slightly more detailed description of its contents.

Our motivation for this work was to understand the existence of Poincaré families on the corresponding coarse moduli schemes, or in other words to decide whether these moduli stacks are neutral as gerbes over their coarse moduli schemes. The consequences for this question are spelled out in [4].

2. The stack of G–bundles and its Picard functor

Here we introduce the basic objects of this paper, namely the moduli stack of principal G–bundles on an algebraic curve and its Picard functor. The main purpose of this section is to fix some notation and terminology; along the way, we record a few basic facts for later use.

2.1. A Picard functor for algebraic stacks. Throughout this paper, we work over an algebraically closed field k. There is no restriction on the characteristic of k. We say that a stack $\mathcal{X}$ over k is *algebraic* if it is an Artin stack and also locally of finite type over k. Every algebraic stack $\mathcal{X} \neq \emptyset$ admits a point $x_0 : \mathrm{Spec}(k) \longrightarrow \mathcal{X}$ according to Hilbert's Nullstellensatz.

A 1–morphism $\Phi : \mathcal{X} \longrightarrow \mathcal{Y}$ of stacks is an *equivalence* if some 1–morphism $\Psi : \mathcal{Y} \longrightarrow \mathcal{X}$ admits 2–isomorphisms $\Psi \circ \Phi \cong \mathrm{id}_{\mathcal{X}}$ and $\Phi \circ \Psi \cong \mathrm{id}_{\mathcal{Y}}$. A diagram

$$\begin{array}{ccc} \mathcal{X} & \xrightarrow{A} & \mathcal{X}' \\ {\scriptstyle\Phi}\downarrow & & \downarrow{\scriptstyle\Phi'} \\ \mathcal{Y} & \xrightarrow{B} & \mathcal{Y}' \end{array}$$

of stacks and 1–morphisms is 2*–commutative* if a 2–isomorphism $\Phi' \circ A \cong B \circ \Phi$ is given. Such a 2–commutative diagram is 2*–cartesian* if the induced 1–morphism from $\mathcal{X}$ to the fibre product of stacks $\mathcal{X}' \times_{\mathcal{Y}'} \mathcal{Y}$ is an equivalence.

Let $\mathcal{X}$ and $\mathcal{Y}$ be algebraic stacks over k. As usual, we denote by $\mathrm{Pic}(\mathcal{X})$ the abelian group of isomorphism classes of line bundles $\mathcal{L}$ on $\mathcal{X}$. If $\mathcal{X} \neq \emptyset$, then

$$\mathrm{pr}_2^* : \mathrm{Pic}(\mathcal{Y}) \longrightarrow \mathrm{Pic}(\mathcal{X} \times \mathcal{Y})$$

is injective because $x_0^* : \mathrm{Pic}(\mathcal{X} \times \mathcal{Y}) \longrightarrow \mathrm{Pic}(\mathcal{Y})$ is a left inverse of pr_2^*.

Definition 2.1.1. The *Picard functor* $\underline{\mathrm{Pic}}(\mathcal{X})$ is the functor from schemes S of finite type over k to abelian groups that sends S to $\mathrm{Pic}(\mathcal{X} \times S)/\,\mathrm{pr}_2^* \mathrm{Pic}(S)$.

If $\underline{\mathrm{Pic}}(\mathcal{X})$ is representable, then we denote the representing scheme again by $\underline{\mathrm{Pic}}(\mathcal{X})$. If $\underline{\mathrm{Pic}}(\mathcal{X})$ is the constant sheaf given by an abelian group Λ, then we say that $\underline{\mathrm{Pic}}(\mathcal{X})$ is *discrete* and simply write $\underline{\mathrm{Pic}}(\mathcal{X}) \cong \Lambda$. (Since the constant Zariski sheaf Λ is already an fppf sheaf, it is not necessary to specify the topology here.)

Lemma 2.1.2. *Let $\mathcal{X}$ and $\mathcal{Y}$ be algebraic stacks over k with* $\Gamma(\mathcal{X}, \mathcal{O}_{\mathcal{X}}) = k$.

i) *The canonical map*

$$\mathrm{pr}_2^* : \Gamma(\mathcal{Y}, \mathcal{O}_{\mathcal{Y}}) \longrightarrow \Gamma(\mathcal{X} \times \mathcal{Y}, \mathcal{O}_{\mathcal{X} \times \mathcal{Y}})$$

is an isomorphism.

ii) *Let $\mathcal{L} \in \mathrm{Pic}(\mathcal{X} \times \mathcal{Y})$ be given. If there is an atlas $u : U \longrightarrow \mathcal{Y}$ for which $u^*\mathcal{L} \in \mathrm{Pic}(\mathcal{X} \times U)$ is trivial, then $\mathcal{L} \in \mathrm{pr}_2^* \mathrm{Pic}(\mathcal{Y})$.*

Proof. i) Since the question is local in $\mathcal{Y}$, we may assume that $\mathcal{Y} = \mathrm{Spec}(A)$ is an affine scheme over k. In this case, we have

$$\Gamma(\mathcal{X} \times \mathcal{Y}, \mathcal{O}_{\mathcal{X}\times\mathcal{Y}}) = \Gamma(\mathcal{X}, (\mathrm{pr}_1)_*\mathcal{O}_{\mathcal{X}\times\mathcal{Y}}) = \Gamma(\mathcal{X}, A \otimes_k \mathcal{O}_{\mathcal{X}}) = A = \Gamma(\mathcal{Y}, \mathcal{O}_{\mathcal{Y}}).$$

ii) Choose a point $x_0 : \mathrm{Spec}(k) \longrightarrow \mathcal{X}$. We claim that $\mathcal{L}$ is isomorphic to $\mathrm{pr}_2^* \mathcal{L}_{x_0}$ for $\mathcal{L}_{x_0} := x_0^*\mathcal{L} \in \mathrm{Pic}(\mathcal{Y})$. More precisely there is a unique isomorphism $\mathcal{L} \cong \mathrm{pr}_2^* \mathcal{L}_{x_0}$ whose restriction to $\{x_0\} \times \mathcal{Y} \cong \mathcal{Y}$ is the identity. To prove this, due to the uniqueness involved, this claim is local in $\mathcal{Y}$. Hence we may assume $\mathcal{Y} = U$, which by assumption means that $\mathcal{L}$ is trivial. In this case, statement (i) implies the claim. □

Corollary 2.1.3. *For $\nu = 1, 2$, let $\mathcal{X}_\nu$ be an algebraic stack over k with $\Gamma(\mathcal{X}_\nu, \mathcal{O}_{\mathcal{X}_\nu}) = k$. Let $\Phi : \mathcal{X}_1 \longrightarrow \mathcal{X}_2$ be a 1–morphism such that the induced morphism of functors $\Phi^* : \underline{\mathrm{Pic}}(\mathcal{X}_2) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{X}_1)$ is injective. Then*

$$\Phi^* : \mathrm{Pic}(\mathcal{X}_2 \times \mathcal{Y}) \longrightarrow \mathrm{Pic}(\mathcal{X}_1 \times \mathcal{Y})$$

is injective for every algebraic stack $\mathcal{Y}$ over k.

Proof. Since $\mathcal{Y}$ is assumed to be locally of finite type over k, we can choose an atlas $u : U \longrightarrow \mathcal{Y}$ such that U is a disjoint union of schemes of finite type over k. Suppose that $\mathcal{L} \in \mathrm{Pic}(\mathcal{X}_2 \times \mathcal{Y})$ has trivial pullback $\Phi^*\mathcal{L} \in \mathrm{Pic}(\mathcal{X}_1 \times \mathcal{Y})$. Then $(\Phi \times u)^*\mathcal{L} \in \mathrm{Pic}(\mathcal{X}_1 \times U)$ is also trivial. Using the assumption on Φ^* it follows that $u^*\mathcal{L} \in \mathrm{Pic}(\mathcal{X}_2 \times U)$ is trivial. Now apply Lemma 2.1.2(ii). □

We will also need the following stacky version of the standard see–saw principle.

Lemma 2.1.4. *Let $\mathcal{X}$ and $\mathcal{Y}$ be two nonempty algebraic stacks over k. If $\underline{\mathrm{Pic}}(\mathcal{X})$ is discrete, and $\Gamma(\mathcal{Y}, \mathcal{O}_{\mathcal{Y}}) = k$, then*

$$\mathrm{pr}_1^* \oplus \mathrm{pr}_2^* : \underline{\mathrm{Pic}}(\mathcal{X}) \oplus \underline{\mathrm{Pic}}(\mathcal{Y}) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{X} \times \mathcal{Y})$$

is an isomorphism of functors.

Proof. Choose points $x_0 : \mathrm{Spec}(k) \longrightarrow \mathcal{X}$ and $y_0 : \mathrm{Spec}(k) \longrightarrow \mathcal{Y}$. The morphism of functors $\mathrm{pr}_1^* \oplus \mathrm{pr}_2^*$ in question is injective, because

$$y_0^* \oplus x_0^* : \underline{\mathrm{Pic}}(\mathcal{X} \times \mathcal{Y}) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{X}) \oplus \underline{\mathrm{Pic}}(\mathcal{Y})$$

is a left inverse of it. Therefore, to prove the lemma it suffices to show that $y_0^* \oplus x_0^*$ is also injective.

So let a scheme S of finite type over k be given, as well as a line bundle $\mathcal{L}$ on $\mathcal{X} \times \mathcal{Y} \times S$ such that $y_0^*\mathcal{L}$ is trivial in $\underline{\mathrm{Pic}}(\mathcal{X})$. We claim that $\mathcal{L}$ is isomorphic to the pullback of a line bundle on $\mathcal{Y} \times S$.

To prove the claim, tensoring $\mathcal{L}$ with an appropriate line bundle on S if necessary, we may assume that $y_0^*\mathcal{L}$ is trivial in $\mathrm{Pic}(\mathcal{X} \times S)$. By assumption,

$\underline{\mathrm{Pic}}(\mathcal{X}) \cong \Lambda$ for some abelian group Λ. Sending any $(y,s) : \mathrm{Spec}(k) \longrightarrow \mathcal{Y} \times S$ to the isomorphism class of

$$(y,s)^*(\mathcal{L}) \in \mathrm{Pic}(\mathcal{X})$$

we obtain a Zariski–locally constant map from the set of k–points in $\mathcal{Y} \times S$ to Λ. This map vanishes on $\{y_0\} \times S$, and hence it vanishes identically on $\mathcal{Y} \times S$ because $\mathcal{Y}$ is connected. This means that $u^*\mathcal{L} \in \mathrm{Pic}(\mathcal{X} \times U)$ is trivial for any atlas $u : U \longrightarrow \mathcal{Y} \times S$. Now Lemma 2.1.2(ii) completes the proof of the claim. If moreover $x_0^*\mathcal{L}$ is trivial in $\underline{\mathrm{Pic}}(\mathcal{Y})$, then $\mathcal{L}$ is even isomorphic to the pullback of a line bundle on S, and hence trivial in $\underline{\mathrm{Pic}}(\mathcal{X} \times \mathcal{Y})$. This proves the injectivity of $y_0^* \oplus x_0^*$, and hence the lemma follows. □

2.2. Principal G–bundles over a curve. We fix an irreducible smooth projective curve C over the algebraically closed base field k. The genus of C will be denoted by g_C. Given a linear algebraic group $G \hookrightarrow \mathrm{GL}_n$, we denote by

$$\mathcal{M}_G$$

the moduli stack of principal G–bundles E on C. More precisely, $\mathcal{M}_G$ is given by the groupoid $\mathcal{M}_G(S)$ of principal G–bundles on $S \times C$ for every k–scheme S. The stack $\mathcal{M}_G$ is known to be algebraic over k (see for example [23, Proposition 3.4], or [24, Théorème 4.6.2.1] together with [29, Lemma 4.8.1]).
Given a morphism of linear algebraic groups $\varphi : G \longrightarrow H$, the extension of the structure group by φ defines a canonical 1–morphism

$$\varphi_* : \mathcal{M}_G \longrightarrow \mathcal{M}_H$$

which more precisely sends a principal G–bundle E to the principal H–bundle

$$\varphi_* E := E \times^G H := (E \times G)/H,$$

following the convention that principal bundles carry a *right* group action. One has a canonical 2–isomorphism $(\psi \circ \varphi)_* \cong \psi_* \circ \varphi_*$ whenever $\psi : H \longrightarrow K$ is another morphism of linear algebraic groups.

Lemma 2.2.1. *Suppose that the diagram of linear algebraic groups*

$$\begin{array}{ccc} H & \xrightarrow{\psi_2} & G_2 \\ {\scriptstyle \psi_1}\downarrow & & \downarrow{\scriptstyle \varphi_2} \\ G_1 & \xrightarrow[\varphi_1]{} & G \end{array}$$

is cartesian. Then the induced 2*–commutative diagram of moduli stacks*

$$\begin{array}{ccc} \mathcal{M}_H & \xrightarrow{(\psi_2)_*} & \mathcal{M}_{G_2} \\ {\scriptstyle (\psi_1)_*}\downarrow & & \downarrow{\scriptstyle (\varphi_2)_*} \\ \mathcal{M}_{G_1} & \xrightarrow[(\varphi_1)_*]{} & \mathcal{M}_G \end{array}$$

is 2*–cartesian.*

Proof. The above 2–commutative diagram defines a 1–morphism

$$\mathcal{M}_H \longrightarrow \mathcal{M}_{G_1} \times_{\mathcal{M}_G} \mathcal{M}_{G_2}.$$

To construct an inverse, let E be a principal G–bundle on some k–scheme X. For $\nu = 1, 2$, let E_ν be a principal G_ν–bundle on X together with an isomorphism $E_\nu \times^{G_\nu} G \cong E$; note that the latter defines a map $E_\nu \longrightarrow E$ of schemes over X. Then $G_1 \times G_2$ acts on $E_1 \times_X E_2$, and the closed subgroup $H \subseteq G_1 \times G_2$ preserves the closed subscheme

$$F := E_1 \times_E E_2 \subseteq E_1 \times_X E_2 \,.$$

This action turns F into a principal H–bundle. Thus we obtain in particular a 1–morphism

$$\mathcal{M}_{G_1} \times_{\mathcal{M}_G} \mathcal{M}_{G_2} \longrightarrow \mathcal{M}_H.$$

It is easy to check that this is the required inverse. □

Let Z be a closed subgroup in the center of G. Then the multiplication $Z \times G \longrightarrow G$ is a group homomorphism; we denote the induced 1–morphism by

$$\_ \otimes \_ : \mathcal{M}_Z \times \mathcal{M}_G \longrightarrow \mathcal{M}_G$$

and call it *tensor product.* In particular, tensoring with a principal Z–bundle ξ on C defines a 1–morphism which we denote by

$$t_\xi : \mathcal{M}_G \longrightarrow \mathcal{M}_G. \tag{1}$$

For commutative G, this tensor product makes $\mathcal{M}_G$ a group stack.
Suppose now that G is reductive. We follow the convention that all reductive groups are smooth and connected. In particular, $\mathcal{M}_G$ is also smooth [3, 4.5.1], so its connected components and its irreducible components coincide; we denote this set of components by $\pi_0(\mathcal{M}_G)$. This set $\pi_0(\mathcal{M}_G)$ can be described as follows; cf. for example [15] or [16].
Let $\iota_G : T_G \hookrightarrow G$ be the inclusion of a maximal torus, with cocharacter group $\Lambda_{T_G} := \mathrm{Hom}(\mathbb{G}_m, T_G)$. Let $\Lambda_{\mathrm{coroots}} \subseteq \Lambda_{T_G}$ be the subgroup generated by the coroots of G. The Weyl group W of (G, T_G) acts on Λ_{T_G}. For every root α with corresponding coroot $\alpha^\vee$, the reflection $s_\alpha \in W$ acts on $\lambda \in \Lambda_{T_G}$ by the formula $s_\alpha(\lambda) = \lambda - \langle \alpha, \lambda \rangle \alpha^\vee$. As the s_α generate W, this implies $w(\lambda) - \lambda \in \Lambda_{\mathrm{coroots}}$ for all $w \in W$ and all $\lambda \in \Lambda_{T_G}$. Thus W acts trivially on $\Lambda_{T_G}/\Lambda_{\mathrm{coroots}}$, so this quotient is, up to a *canonical* isomorphism, independent of the choice of T_G. We denote this quotient by $\pi_1(G)$; if $\pi_1(G)$ is trivial, then G is called simply connected. For $k = \mathbb{C}$, these definitions coincide with the usual notions for the topological space $G(\mathbb{C})$.
Sending each line bundle on C to its degree we define an isomorphism $\pi_0(\mathcal{M}_{\mathbb{G}_m}) \longrightarrow \mathbb{Z}$, which induces an isomorphism $\pi_0(\mathcal{M}_{T_G}) \longrightarrow \Lambda_{T_G}$. Its inverse, composed with the map

$$(\iota_G)_* : \pi_0(\mathcal{M}_{T_G}) \longrightarrow \pi_0(\mathcal{M}_G)\,,$$

is known to induce a canonical bijection

$$\pi_1(G) = \Lambda_{T_G}/\Lambda_{\mathrm{coroots}} \xrightarrow{\sim} \pi_0(\mathcal{M}_G),$$

cf. [10] and [16]. We denote by $\mathcal{M}_G^d$ the component of $\mathcal{M}_G$ given by $d \in \pi_1(G)$.

Lemma 2.2.2. *Let $\varphi : G \twoheadrightarrow H$ be an epimorphism of reductive groups over k whose kernel is contained in the center of G. For each $d \in \pi_1(G)$, the 1–morphism*

$$\varphi_* : \mathcal{M}_G^d \longrightarrow \mathcal{M}_H^e, \qquad e := \varphi_*(d) \in \pi_1(H),$$

is faithfully flat.

Proof. Let $T_H \subseteq H$ be the image of the maximal torus $T_G \subseteq G$. Let $B_G \subseteq G$ be a Borel subgroup containing T_G; then

$$B_H := \varphi(B_G) \subset H$$

is a Borel subgroup of H containing T_H. For the moment, we denote

- by $\mathcal{M}_{T_G}^d \subseteq \mathcal{M}_{T_G}$ and $\mathcal{M}_{B_G}^d \subseteq \mathcal{M}_{B_G}$ the inverse images of $\mathcal{M}_G^d \subseteq \mathcal{M}_G$, and
- by $\mathcal{M}_{T_H}^e \subseteq \mathcal{M}_{T_H}$ and $\mathcal{M}_{B_H}^e \subseteq \mathcal{M}_{B_H}$ the inverse images of $\mathcal{M}_H^e \subseteq \mathcal{M}_H$.

Let $\pi_G : B_G \twoheadrightarrow T_G$ and $\pi_H : B_H \twoheadrightarrow T_H$ denote the canonical surjections. Then

$$\mathcal{M}_{B_G}^d = (\pi_G)_*^{-1}(\mathcal{M}_{T_G}^d) \qquad \text{and} \qquad \mathcal{M}_{B_H}^e = (\pi_H)_*^{-1}(\mathcal{M}_{T_H}^e),$$

because $\pi_0(\mathcal{M}_{T_G}) = \pi_0(\mathcal{M}_{B_G})$ and $\pi_0(\mathcal{M}_{T_H}) = \pi_0(\mathcal{M}_{B_H})$ according to the proof of [10, Proposition 5]. Applying Lemma 2.2.1 to the two cartesian squares

$$\begin{array}{ccccc} T_G & \xleftarrow{\pi_G} & B_G & \hookrightarrow & G \\ \downarrow{\scriptstyle \varphi_T} & & \downarrow{\scriptstyle \varphi_B} & & \downarrow{\scriptstyle \varphi} \\ T_H & \xleftarrow{\pi_H} & B_H & \hookrightarrow & H \end{array}$$

of groups, we get two 2–cartesian squares

$$\begin{array}{ccccc} \mathcal{M}_{T_G}^d & \longleftarrow & \mathcal{M}_{B_G}^d & \longrightarrow & \mathcal{M}_G^d \\ \downarrow{\scriptstyle (\varphi_T)_*} & & \downarrow{\scriptstyle (\varphi_B)_*} & & \downarrow{\scriptstyle \varphi_*} \\ \mathcal{M}_{T_H}^e & \longleftarrow & \mathcal{M}_{B_H}^e & \longrightarrow & \mathcal{M}_H^e \end{array}$$

of moduli stacks. Since $(\varphi_T)_*$ is faithfully flat, its pullback $(\varphi_B)_*$ is so as well. This implies that φ_* is also faithfully flat, as some open substack of $\mathcal{M}_{B_H}^e$ maps smoothly and surjectively onto $\mathcal{M}_H^e$, according to [10, Propositions 1 and 2]. □

3. The case of torus

This section deals with the Picard functor of the moduli stack $\mathcal{M}_G^0$ in the special case where $G = T$ is a torus. We explain in the second subsection that its description involves the character group $\mathrm{Hom}(T, \mathbb{G}_m)$ and the Picard functor of its coarse moduli scheme, which is isomorphic to a product of copies of the Jacobian J_C. As a preparation, the first subsection deals with the Néron–Severi group of such products of principally polarised abelian varieties. A little care is required to keep everything functorial in T, since this functoriality will be needed later.

3.1. ON PRINCIPALLY POLARISED ABELIAN VARIETIES. Let A be an abelian variety over k, with dual abelian variety $A^\vee$ and Néron–Severi group

$$\mathrm{NS}(A) := \mathrm{Pic}(A)/A^\vee(k)\,.$$

For a line bundle L on A, the standard morphism

$$\phi_L : A \longrightarrow A^\vee$$

sends $a \in A(k)$ to $\tau_a^*(L) \otimes L^{\mathrm{dual}}$ where $\tau_a : A \longrightarrow A$ is the translation by a. ϕ_L is a homomorphism by the theorem of the cube [27, §6]. Let a principal polarisation

$$\phi : A \xrightarrow{\sim} A^\vee$$

be given. Let

$$c^\phi : \mathrm{NS}(A) \longrightarrow \mathrm{End}\, A$$

be the injective homomorphism that sends the class of L to $\phi^{-1} \circ \phi_L$. We denote by $\dagger : \mathrm{End}\, A \longrightarrow \mathrm{End}\, A$ the Rosati involution associated to ϕ; so by definition, it sends $\alpha : A \longrightarrow A$ to $\alpha^\dagger := \phi^{-1} \circ \alpha^\vee \circ \phi$.

LEMMA 3.1.1. *An endomorphism $\alpha \in \mathrm{End}(A)$ is in the image of c^ϕ if and only if $\alpha^\dagger = \alpha$.*

Proof. If $k = \mathbb{C}$, this is contained in [21, Chapter 5, Proposition 2.1]. For polarisations of arbitrary degree, the analogous statement about $\mathrm{End}(A) \otimes \mathbb{Q}$ is shown in [27, p. 190]; its proof carries over to the situation of this lemma as follows.

Let l be a prime number, $l \neq \mathrm{char}(k)$, and let

$$e_l : T_l(A) \times T_l(A^\vee) \longrightarrow \mathbb{Z}_l(1)$$

be the standard pairing between the Tate modules of A and $A^\vee$, cf. [27, §20]. According to [27, §20, Theorem 2 and §23, Theorem 3], a homomorphism $\psi : A \longrightarrow A^\vee$ is of the form $\psi = \phi_L$ for some line bundle L on A if and only if

$$e_l(x, \psi_* y) = -e_l(y, \psi_* x) \quad \text{for all} \quad x, y \in T_l(A)\,.$$

In particular, this holds for ϕ. Hence the right hand side equals

$$-e_l(y, \psi_* x) = -e_l(y, \phi_* \phi_*^{-1} \psi_* x) = e_l(\phi_*^{-1} \psi_* x, \phi_* y) = e_l(x, \psi_*^\vee (\phi^{-1})_*^\vee \phi_* y)\,,$$

where the last equality follows from [27, p. 186, equation (I)]. Since the pairing e_l is nondegenerate, it follows that $\psi = \phi_L$ holds for some L if and only if

$$\psi_* y = \psi_*^\vee (\phi^{-1})_*^\vee \phi_* y \quad \text{for all} \quad y \in T_l(A)\,,$$

hence if and only if $\psi = \psi^\vee \circ (\phi^{-1})^\vee \circ \phi$. By definition of the Rosati involution $\dagger$, the latter is equivalent to $(\phi^{-1} \circ \psi)^\dagger = \phi^{-1} \circ \psi$. □

Let Λ be a finitely generated free abelian group. Let $\Lambda \otimes A$ denote the abelian variety over k with group of S–valued points $\Lambda \otimes A(S)$ for any k–scheme S.

Definition 3.1.2. The subgroup

$$\mathrm{Hom}^s(\Lambda \otimes \Lambda, \operatorname{End} A) \subseteq \mathrm{Hom}(\Lambda \otimes \Lambda, \operatorname{End} A)$$

consists of all $b : \Lambda \otimes \Lambda \longrightarrow \operatorname{End} A$ with $b(\lambda_1 \otimes \lambda_2)^\dagger = b(\lambda_2 \otimes \lambda_1)$ for all $\lambda_1, \lambda_2 \in \Lambda$.

Corollary 3.1.3. *There is a unique isomorphism*

$$c_\Lambda^\phi : \mathrm{NS}(\Lambda \otimes A) \xrightarrow{\sim} \mathrm{Hom}^s(\Lambda \otimes \Lambda, \operatorname{End} A)$$

which sends the class of each line bundle L on $\Lambda \otimes A$ to the linear map

$$c_\Lambda^\phi(L) : \Lambda \otimes \Lambda \longrightarrow \operatorname{End} A$$

defined by sending $\lambda_1 \otimes \lambda_2$ for $\lambda_1, \lambda_2 \in \Lambda$ to the composition

$$A \xrightarrow{\lambda_1 \otimes \_} \Lambda \otimes A \xrightarrow{\phi_L} (\Lambda \otimes A)^\vee \xrightarrow{(\lambda_2 \otimes \_)^\vee} A^\vee \xrightarrow{\phi^{-1}} A.$$

Proof. The uniqueness is clear. For the existence, we may then choose an isomorphism $\Lambda \cong \mathbb{Z}^r$; it yields an isomorphism $\Lambda \otimes A \cong A^r$. Let

$$\phi^r = \underbrace{\phi \times \cdots \times \phi}_{r \text{ factors}} : A^r \xrightarrow{\sim} (A^\vee)^r = (A^r)^\vee$$

be the diagonal principal polarisation on A^r. According to Lemma 3.1.1,

$$c^{\phi^r} : \mathrm{NS}(A^r) \longrightarrow \operatorname{End}(A^r)$$

is an isomorphism onto the Rosati–invariants. Under the standard isomorphisms

$$\operatorname{End}(A^r) = \mathrm{Mat}_{r\times r}(\operatorname{End} A) = \mathrm{Hom}(\mathbb{Z}^r \otimes \mathbb{Z}^r, \operatorname{End} A),$$

the Rosati involution on $\operatorname{End}(A^r)$ corresponds to the involution $(\alpha_{ij}) \longmapsto (\alpha_{ji}^\dagger)$ on $\mathrm{Mat}_{r\times r}(\operatorname{End} A)$, and hence the Rosati–invariant part of $\operatorname{End}(A^r)$ corresponds to $\mathrm{Hom}^s(\mathbb{Z}^r \otimes \mathbb{Z}^r, \operatorname{End} A)$. Thus we obtain an isomorphism

$$\mathrm{NS}(\Lambda \otimes A) \cong \mathrm{NS}(A^r) \xrightarrow{c^{\phi^r}} \mathrm{Hom}^s(\mathbb{Z}^r \otimes \mathbb{Z}^r, \operatorname{End} A) \cong \mathrm{Hom}^s(\Lambda \otimes \Lambda, \operatorname{End} A).$$

By construction, it maps the class of each line bundle L on $\Lambda \otimes A$ to the map $c_\Lambda^\phi(L) : \Lambda \otimes \Lambda \longrightarrow \operatorname{End} A$ prescribed above. □

3.2. Line bundles on $\mathcal{M}_T^0$. Let $T \cong \mathbb{G}_m^r$ be a torus over k. We will always denote by

$$\Lambda_T := \mathrm{Hom}(\mathbb{G}_m, T)$$

the cocharacter lattice. We set in the previous subsection this finitely generated free abelian group and the Jacobian variety J_C, endowed with the principal polarisation $\phi_\Theta : J_C \xrightarrow{\sim} J_C^\vee$ given by the autoduality of J_C. Recall that ϕ_Θ comes from a line bundle $\mathcal{O}(\Theta)$ on J_C corresponding to a theta divisor $\Theta \subseteq J_C$.

Definition 3.2.1. The finitely generated free abelian group

$$\mathrm{NS}(\mathcal{M}_T) := \mathrm{Hom}(\Lambda_T, \mathbb{Z}) \oplus \mathrm{Hom}^s(\Lambda_T \otimes \Lambda_T, \operatorname{End} J_C)$$

is the *Néron–Severi group* of $\mathcal{M}_T$.

For each finitely generated abelian group Λ, we denote by $\underline{\mathrm{Hom}}(\Lambda, J_C)$ the k–scheme of homomorphisms from Λ to J_C. If $\Lambda \cong \mathbb{Z}^r \times \mathbb{Z}/n_1 \times \cdots \times \mathbb{Z}/n_s$, then

$$\underline{\mathrm{Hom}}(\Lambda, J_C) \cong J_C^r \times J_C[n_1] \times \cdots \times J_C[n_s]$$

where $J_C[n]$ denotes the kernel of the map $J_C \longrightarrow J_C$ defined by multiplication with n.

Proposition 3.2.2. i) *The Picard functor $\underline{\mathrm{Pic}}(\mathcal{M}_T^0)$ is representable by a scheme locally of finite type over k.*

ii) *There is a canonical exact sequence of commutative group schemes*

$$0 \longrightarrow \underline{\mathrm{Hom}}(\Lambda_T, J_C) \xrightarrow{j_T} \underline{\mathrm{Pic}}(\mathcal{M}_T^0) \xrightarrow{c_T} \mathrm{NS}(\mathcal{M}_T) \longrightarrow 0.$$

iii) *Let ξ be a principal T–bundle of degree $0 \in \Lambda_T$ on C. Then the diagram*

$$\begin{array}{ccccccccc} 0 & \longrightarrow & \underline{\mathrm{Hom}}(\Lambda_T, J_C) & \xrightarrow{j_T} & \underline{\mathrm{Pic}}(\mathcal{M}_T^0) & \xrightarrow{c_T} & \mathrm{NS}(\mathcal{M}_T) & \longrightarrow & 0 \\ & & \| & & \downarrow{\scriptstyle t_\xi^*} & & \| & & \\ 0 & \longrightarrow & \underline{\mathrm{Hom}}(\Lambda_T, J_C) & \xrightarrow{j_T} & \underline{\mathrm{Pic}}(\mathcal{M}_T^0) & \xrightarrow{c_T} & \mathrm{NS}(\mathcal{M}_T) & \longrightarrow & 0 \end{array}$$

commutes.

Proof. Let a line bundle $\mathcal{L}$ on $\mathcal{M}_T^0$ be given. Consider the point in $\mathcal{M}_T^0$ given by a principal T–bundle ξ on C of degree $0 \in \Lambda_T$. The fiber of $\mathcal{L}_\xi$ at this point is a 1-dimensional vector space $\mathcal{L}_\xi$, endowed with a group homomorphism

$$w(\mathcal{L})_\xi : T = \mathrm{Aut}(\xi) \longrightarrow \mathrm{Aut}(\mathcal{L}_\xi) = \mathbb{G}_m$$

since $\mathcal{L}$ is a line bundle on the stack. As $\mathcal{M}_T^0$ is connected, the character $w(\mathcal{L})_\xi$ is independent of ξ; we denote it by

$$w(\mathcal{L}) : T \longrightarrow \mathbb{G}_m$$

and call it the *weight* $w(\mathcal{L})$ of $\mathcal{L}$. Let

$$q : \mathcal{M}_T^0 \longrightarrow \mathfrak{M}_T^0$$

be the canonical morphism to the coarse moduli scheme $\mathfrak{M}_T^0$, which is an abelian variety canonically isomorphic to $\underline{\mathrm{Hom}}(\Lambda_T, J_C)$. Line bundles of weight 0 on $\mathcal{M}_T^0$ descend to $\mathfrak{M}_T^0$, so the sequence

$$0 \longrightarrow \mathrm{Pic}(\mathfrak{M}_T^0) \xrightarrow{q^*} \mathrm{Pic}(\mathcal{M}_T^0) \xrightarrow{w} \mathrm{Hom}(\Lambda_T, \mathbb{Z})$$

is exact. This extends for families. Since $\underline{\mathrm{Pic}}(A)$ is representable for any abelian variety A, the proof of (i) is now complete.

Standard theory of abelian varieties and Corollary 3.1.3 together yield another short exact sequence

$$0 \longrightarrow \underline{\mathrm{Hom}}(\Lambda_T, J_C) \longrightarrow \underline{\mathrm{Pic}}(\mathfrak{M}_T^0) \longrightarrow \mathrm{Hom}^s(\Lambda_T \otimes \Lambda_T, \mathrm{End}\, J_C) \longrightarrow 0\,.$$

Given a character $\chi : T \longrightarrow \mathbb{G}_m$ and $p \in C(k)$, we denote by $\chi_* \mathcal{L}_p^{\mathrm{univ}}$ the line bundle on $\mathcal{M}_T^0$ that associates to each T–bundle L on C the $\mathbb{G}_m$–bundle $\chi_* L_p$.

Clearly, $\chi_*\mathcal{L}_p^{\text{univ}}$ has weight χ; in particular, it follows that w is surjective, so we get an exact sequence of discrete abelian groups

$$0 \longrightarrow \operatorname{Hom}^s(\Lambda_T \otimes \Lambda_T, \operatorname{End} J_C) \longrightarrow \underline{\operatorname{Pic}}(\mathcal{M}_T^0)/\underline{\operatorname{Hom}}(\Lambda_T, J_C) \longrightarrow \operatorname{Hom}(\Lambda_T, \mathbb{Z}) \longrightarrow 0\,.$$

Since C is connected, the algebraic equivalence class of $\chi_*\mathcal{L}_p^{\text{univ}}$ does not depend on the choice of p; sending χ to the class of $\chi_*\mathcal{L}_p^{\text{univ}}$ thus defines a canonical splitting of the latter exact sequence. This proves (ii).

Finally, it is standard that t_ξ^* (see (1)) is the identity map on $\underline{\operatorname{Pic}}^0(\mathfrak{M}_T^0) = \underline{\operatorname{Hom}}(\Lambda, J_C)$ (see [26, Proposition 9.2]), and t_ξ^* induces the identity map on the discrete quotient $\underline{\operatorname{Pic}}(\mathcal{M}_T^0)/\underline{\operatorname{Pic}}^0(\mathfrak{M}_T^0)$ because ξ can be connected to the trivial T–bundle in $\mathcal{M}_T^0$. ☐

Remark 3.2.3. The exact sequence in Proposition 3.2.2(ii) is functorial in T. More precisely, each homomorphism of tori $\varphi : T \longrightarrow T'$ induces a morphism of exact sequences

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \underline{\operatorname{Hom}}(\Lambda_{T'}, J_C) & \xrightarrow{j_{T'}} & \underline{\operatorname{Pic}}(\mathcal{M}_{T'}^0) & \xrightarrow{c_{T'}} & \operatorname{NS}(\mathcal{M}_{T'}) & \longrightarrow & 0 \\
 & & \downarrow{\scriptstyle\varphi^*} & & \downarrow{\scriptstyle\varphi^*} & & \downarrow{\scriptstyle\varphi^*} & & \\
0 & \longrightarrow & \underline{\operatorname{Hom}}(\Lambda_T, J_C) & \xrightarrow{j_T} & \underline{\operatorname{Pic}}(\mathcal{M}_T^0) & \xrightarrow{c_T} & \operatorname{NS}(\mathcal{M}_T) & \longrightarrow & 0.
\end{array}$$

Corollary 3.2.4. *Let T_1 and T_2 be tori over k. Then*

$$\operatorname{pr}_1^* \oplus \operatorname{pr}_2^* : \underline{\operatorname{Pic}}(\mathcal{M}_{T_1}^0) \oplus \underline{\operatorname{Pic}}(\mathcal{M}_{T_2}^0) \longrightarrow \underline{\operatorname{Pic}}(\mathcal{M}_{T_1 \times T_2}^0)$$

is a closed immersion of commutative group schemes over k.

Proof. As before, let Λ_{T_1}, Λ_{T_2} and $\Lambda_{T_1 \times T_2}$ denote the cocharacter lattices. Then

$$\operatorname{pr}_1^* \oplus \operatorname{pr}_2^* : \underline{\operatorname{Hom}}(\Lambda_{T_1}, J_C) \oplus \underline{\operatorname{Hom}}(\Lambda_{T_2}, J_C) \longrightarrow \underline{\operatorname{Hom}}(\Lambda_{T_1 \times T_2}, J_C)$$

is an isomorphism, and the homomorphism of discrete abelian groups

$$\operatorname{pr}_1^* \oplus \operatorname{pr}_2^* : \operatorname{NS}(\mathcal{M}_{T_1}) \oplus \operatorname{NS}(\mathcal{M}_{T_2}) \longrightarrow \operatorname{NS}(\mathcal{M}_{T_1 \times T_2})$$

is injective by Definition 3.2.1. ☐

4. The twisted simply connected case

Throughout most of this section, the reductive group G over k will be simply connected. Using the work of Faltings [13] on the Picard functor of $\mathcal{M}_G$, we describe here the Picard functor of the twisted moduli stacks $\mathcal{M}_{\widehat{G},L}$ introduced in [2]. In the case $G = \mathrm{SL}_n$, these are moduli stacks of vector bundles with fixed determinant; their construction in general is recalled in Subsection 4.2 below.

The result, proved in that subsection as Proposition 4.2.3, is essentially the same: for almost simple G, line bundles on $\mathcal{M}_{\widehat{G},L}$ are classified by an integer, their so–called central charge. The main tool for that are as usual algebraic loop groups; what we need about them is collected in Subsection 4.1.

For later use, we need to keep track of the functoriality in G, in particular of the pullback to a maximal torus T_G in G. To state this more easily, we translate the central charge into a Weyl–invariant symmetric bilinear form on the cocharacter lattice of T_G, replacing each integer by the corresponding multiple of the basic inner product. This allows to describe the pullback to T_G in Proposition 4.4.7(iii). Along the way, we also consider the pullback along representations of G; these just correspond to the pullback of bilinear forms, which reformulates — and generalises to arbitrary characteristic — the usual multiplication by the Dynkin index [20]. Subsection 4.3 describes these pullback maps combinatorially in terms of the root system, and Subsection 4.4 proves that these combinatorial maps actually give the pullback of line bundles on these moduli stacks.

4.1. Loop groups. Let G be a reductive group over k. We denote

- by LG the algebraic loop group of G, meaning the group ind–scheme over k whose group of A–valued points for any k–algebra A is $G(A((t)))$,
- by $L^+G \subseteq LG$ the subgroup with A–valued points $G(A[[t]]) \subseteq G(A((t)))$,
- and for $n \geq 1$, by $L^{\geq n}G \subseteq L^+G$ the kernel of the reduction modulo t^n.

Note that L^+G and $L^{\geq n}G$ are affine group schemes over k. The k-algebra corresponding to $L^{\geq n}G$ is the inductive limit over all $N > n$ of the k–algebras corresponding to $L^{\geq n}G/L^{\geq N}$. A similar statement holds for L^+G.
If X is anything defined over k, let X_S denote its pullback to a k–scheme S.

Lemma 4.1.1. *Let S be a reduced scheme over k. For $n \geq 1$, every morphism $\varphi : (L^{\geq n}G)_S \longrightarrow (\mathbb{G}_m)_S$ of group schemes over S is trivial.*

Proof. This follows from the fact that $L^{\geq n}G$ is pro–unipotent; more precisely: As S is reduced, the claim can be checked on geometric points $\mathrm{Spec}(k') \longrightarrow S$. Replacing k by the larger algebraically closed field k' if necessary, we may thus assume $S = \mathrm{Spec}(k)$; then φ is a morphism $L^{\geq n}G \longrightarrow \mathbb{G}_m$.
Since the k–algebra corresponding to $\mathbb{G}_m$ is finitely generated, it follows that φ factors through $L^{\geq n}G/L^{\geq N}G$ for some $N > n$. Denoting by $\mathfrak{g}$ the Lie algebra of G, [8, II, §4, Theorem 3.5] provides an exact sequence

$$1 \longrightarrow L^{\geq N}G \longrightarrow L^{\geq N-1}G \longrightarrow \mathfrak{g} \longrightarrow 1.$$

Thus the restriction of φ to $L^{\geq N-1}G$ induces a character on the additive group scheme underlying $\mathfrak{g}$. Hence this restriction has to vanish, so φ also factors through $L^{\geq n}G/L^{\geq N-1}G$. Iterating this argument shows that φ is trivial. □

Lemma 4.1.2. *Suppose that the reductive group G is simply connected, in particular semisimple. If a central extension of group schemes over k*

$$1 \longrightarrow \mathbb{G}_m \longrightarrow \mathcal{H} \xrightarrow{\pi} L^+G \longrightarrow 1 \tag{2}$$

splits over $L^{\geq n}G$ for some $n \geq 1$, then it splits over L^+G.

Proof. Let a splitting over $L^{\geq n}G$ be given, i.e. a homomorphism of group schemes $\sigma : L^{\geq n}G \longrightarrow \mathcal{H}$ such that $\pi \circ \sigma = \mathrm{id}$. Given points $h \in \mathcal{H}(S)$ and $g \in L^{\geq n}G(S)$ for some k-scheme S, the two elements

$$h \cdot \sigma(g) \cdot h^{-1} \qquad \text{and} \qquad \sigma(\pi(h) \cdot g \cdot \pi(h)^{-1})$$

in $\mathcal{H}(S)$ have the same image under π, so their difference is an element in $\mathbb{G}_m(S)$, which we denote by $\varphi_h(g)$. Sending h and g to h and $\varphi_h(g)$ defines a morphism

$$\varphi : (L^{\geq n}G)_{\mathcal{H}} \longrightarrow (\mathbb{G}_m)_{\mathcal{H}}$$

of group schemes over $\mathcal{H}$. Since $L^+G/L^{\geq 1}G \cong G$ and $L^{\geq N-1}G/L^{\geq N} \cong \mathfrak{g}$ for $N \geq 2$ are smooth, their successive extension $L^+G/L^{\geq N}G$ is also smooth. Thus the limit L^+G is reduced, so $\mathcal{H}$ is reduced as well. Using the previous lemma, it follows that φ is the constant map 1; in other words, σ commutes with conjugation. σ is a closed immersion because $\pi \circ \sigma$ is, so σ is an isomorphism onto a closed normal subgroup, and the quotient is a central extension

$$1 \longrightarrow \mathbb{G}_m \longrightarrow \mathcal{H}/\sigma(L^{\geq n}G) \longrightarrow L^+G/L^{\geq n}G \longrightarrow 1.$$

If $n \geq 2$, then this restricts to a central extension of $L^{\geq n-1}G/L^{\geq n}G \cong \mathfrak{g}$ by $\mathbb{G}_m$. It can be shown that any such extension splits.
(Indeed, the unipotent radical of the extension projects isomorphically to the quotient $\mathfrak{g}$. Note that the unipotent radical does not intersect the subgroup $\mathbb{G}_m$, and the quotient by the subgroup generated by the unipotent radical and $\mathbb{G}_m$ is reductive, so this this reductive quotient being a quotient of $\mathfrak{g}$ is in fact trivial.)
Therefore, the image of a section $\mathfrak{g} \longrightarrow \mathcal{H}/\sigma(L^{\geq n}G)$ has an inverse image in $\mathcal{H}$ which π maps isomorphically onto $L^{\geq n-1}G \subseteq L^+G$. Hence the given central extension (2) splits over $L^{\geq n-1}G$ as well. Repeating this argument, we get a splitting over $L^{\geq 1}G$, and finally also over L^+G, because every central extension of $L^+G/L^{\geq 1}G \cong G$ by $\mathbb{G}_m$ splits as well, G being simply connected.
(To prove the last assertion, for any extension $\widetilde{G}$ of G by $\mathbb{G}_m$, consider the commutator subgroup $[\widetilde{G}, \widetilde{G}]$ of $\widetilde{G}$. It projects surjectively to the commutator subgroup of G which is G itself. Since $[\widetilde{G}, \widetilde{G}]$ is connected and reduced, and G is simply connected, this surjective morphism must be an isomorphism.) □

4.2. Descent from the affine Grassmannian. Let G be a reductive group over k. We denote by Gr_G the affine Grassmannian of G, i.e. the quotient LG/L^+G in the category of fppf–sheaves. Let $\widehat{\mathcal{O}}_{C,p}$ denote the completion of the local ring $\mathcal{O}_{C,p}$ of the scheme C in a point $p \in C(k)$. Given a uniformising element $z \in \widehat{\mathcal{O}}_{C,p}$, there is a standard 1–morphism

$$\mathrm{glue}_{p,z} : \mathrm{Gr}_G \longrightarrow \mathcal{M}_G$$

that sends each coset $f \cdot L^+G$ to the trivial G–bundles over $C \backslash \{p\}$ and over $\widehat{\mathcal{O}}_{C,p}$, glued by the automorphism $f(z)$ of the trivial G–bundle over the intersection; cf. for example [23, Section 3], [13, Corollary 16], or [14, Proposition 3].

For the rest of this subsection, we assume that G is simply connected, hence semisimple. In this case, Gr_G is known to be an ind–scheme over k. More precisely, [13, Theorem 8] implies that Gr_G is an inductive limit of projective Schubert varieties over k, which are reduced and irreducible. Thus the canonical map

$$\mathrm{pr}_2^* : \Gamma(S, \mathcal{O}_S) \longrightarrow \Gamma(\mathrm{Gr}_G \times S, \mathcal{O}_{\mathrm{Gr}_G \times S}) \tag{3}$$

is an isomorphism for every scheme S of finite type over k.
Define the Picard functor $\underline{\mathrm{Pic}}(\mathrm{Gr}_G)$ from schemes of finite type over k to abelian groups as in definition 2.1.1. The following theorem about it is proved in full generality in [13]. Over $k = \mathbb{C}$, the group $\mathrm{Pic}(\mathrm{Gr}_G)$ is also determined in [25] as well as in [20], and $\mathrm{Pic}(\mathcal{M}_G)$ is determined in [23] together with [30].

Theorem 4.2.1 (Faltings). *Let G be simply connected and almost simple.*

i) $\underline{\mathrm{Pic}}(\mathrm{Gr}_G) \cong \mathbb{Z}$.
ii) $\mathrm{glue}_{p,z}^* : \underline{\mathrm{Pic}}(\mathcal{M}_G) \longrightarrow \underline{\mathrm{Pic}}(\mathrm{Gr}_G)$ *is an isomorphism of functors.*

The purpose of this subsection is to carry part (ii) over to twisted moduli stacks in the sense of [2]; cf. also the first remark on page 67 of [13]. More precisely, let an exact sequence of reductive groups

$$1 \longrightarrow G \longrightarrow \widehat{G} \xrightarrow{\mathrm{dt}} \mathbb{G}_m \longrightarrow 1 \tag{4}$$

be given, and a line bundle L on C. We denote by $\mathcal{M}_{\widehat{G},L}$ the moduli stack of principal $\widehat{G}$–bundles E on C together with an isomorphism $\mathrm{dt}_* E \cong L$; cf. section 2 of [2]. If for example the given exact sequence is

$$1 \longrightarrow \mathrm{SL}_n \longrightarrow \mathrm{GL}_n \xrightarrow{\det} \mathbb{G}_m \longrightarrow 1,$$

then $\mathcal{M}_{\mathrm{GL}_n,L}$ is the moduli stack of vector bundles with fixed determinant L. In general, the stack $\mathcal{M}_{\widehat{G},L}$ comes with a 2–cartesian diagram

$$\begin{array}{ccc} \mathcal{M}_{\widehat{G},L} & \longrightarrow & \mathcal{M}_{\widehat{G}} \\ \downarrow & & \downarrow{\scriptstyle \mathrm{dt}_*} \\ \mathrm{Spec}(k) & \xrightarrow{L} & \mathcal{M}_{\mathbb{G}_m} \end{array}$$

from which we see in particular that $\mathcal{M}_{\widehat{G},L}$ is algebraic. It satisfies the following variant of the Drinfeld–Simpson uniformisation theorem [10, Theorem 3].

Lemma 4.2.2. *Let a point $p \in C(k)$ and a principal $\widehat{G}$–bundle $\mathcal{E}$ on $C \times S$ for some k–scheme S be given. Every trivialisation of the line bundle $\mathrm{dt}_* \mathcal{E}$ over $(C \setminus \{p\}) \times S$ can étale–locally in S be lifted to a trivialisation of $\mathcal{E}$ over $(C \setminus \{p\}) \times S$.*

Proof. The proof in [10] carries over to this situation as follows. Choose a maximal torus $T_{\widehat{G}} \subseteq \widehat{G}$. Using [10, Theorem 1], we may assume that $\mathcal{E}$ comes from a principal $T_{\widehat{G}}$–bundle; cf. the first paragraph in the proof of [10, Theorem 3]. Arguing as in the third paragraph of that proof, we may change this principal

$T_{\widehat{G}}$–bundle by the extension of $\mathbb{G}_m$–bundles along coroots $\mathbb{G}_m \longrightarrow T_{\widehat{G}}$. Since simple coroots freely generate the kernel T_G of $T_{\widehat{G}} \twoheadrightarrow \mathbb{G}_m$, we can thus achieve that this $T_{\widehat{G}}$–bundle is trivial over $(C \setminus \{p\}) \times S$. Because $\mathbb{G}_m$ is a direct factor of $T_{\widehat{G}}$, we can hence lift the given trivialisation to the $T_{\widehat{G}}$–bundle, and hence also to $\mathcal{E}$. □

Let $d \in \mathbb{Z}$ be the degree of L. Since dt in (4) maps the (reduced) identity component $Z^0 \cong \mathbb{G}_m$ of the center in $\widehat{G}$ surjectively onto $\mathbb{G}_m$, there is a Z^0–bundle ξ (of degree 0) on C with $\mathrm{dt}_*(\xi) \otimes \mathcal{O}_C(dp) \cong L$; tensoring with it defines an equivalence

$$t_\xi : \mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)} \xrightarrow{\sim} \mathcal{M}_{\widehat{G},L}.$$

Choose a homomorphism $\delta : \mathbb{G}_m \longrightarrow \widehat{G}$ with $\mathrm{dt} \circ \delta = d \in \mathbb{Z} = \mathrm{Hom}(\mathbb{G}_m, \mathbb{G}_m)$. We denote by $t^\delta \in L\widehat{G}(k)$ the image of the tautological loop $t \in L\mathbb{G}_m(k)$ under $\delta_* : L\mathbb{G}_m \longrightarrow L\widehat{G}$. The map

$$t^\delta \cdot \_ : \mathrm{Gr}_G \longrightarrow \mathrm{Gr}_{\widehat{G}}$$

sends, for each point f in LG, the coset $f \cdot L^+G$ to the coset $t^\delta f \cdot L^+\widehat{G}$. Its composition $\mathrm{Gr}_G \longrightarrow \mathcal{M}_{\widehat{G}}$ with $\mathrm{glue}_{p,z}$ factors naturally through a 1–morphism

$$\mathrm{glue}_{p,z,\delta} : \mathrm{Gr}_G \longrightarrow \mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)},$$

because $\mathrm{dt}_* \circ (t^\delta \cdot \_) : LG \longrightarrow L\widehat{G} \longrightarrow L\mathbb{G}_m$ is the constant map t^d, which via gluing yields the line bundle $\mathcal{O}_C(dp)$. Lemma 4.2.2 provides local sections of $\mathrm{glue}_{p,z,\delta}$. These show in particular that

$$\mathrm{glue}^*_{p,z,\delta} : \Gamma(\mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)}, \mathcal{O}_{\mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)}}) \longrightarrow \Gamma(\mathrm{Gr}_G, \mathcal{O}_{\mathrm{Gr}_G})$$

is injective. Hence both spaces of sections contain only the constants, since $\Gamma(\mathrm{Gr}_G, \mathcal{O}_{\mathrm{Gr}_G}) = k$ by equation (3). Using the above equivalence t_ξ, this implies

$$\Gamma(\mathcal{M}_{\widehat{G},L}, \mathcal{O}_{\mathcal{M}_{\widehat{G},L}}) = k\,. \tag{5}$$

Proposition 4.2.3. *Let G be simply connected and almost simple. Then*

$$\mathrm{glue}^*_{p,z,\delta} : \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)}) \longrightarrow \underline{\mathrm{Pic}}(\mathrm{Gr}_G)$$

is an isomorphism of functors.

Proof. LG acts on Gr_G by multiplication from the left. Embedding the k–algebra $\mathcal{O}_{C\setminus p} := \Gamma(C \setminus \{p\}, \mathcal{O}_C)$ into $k((t))$ via the Laurent development at p in the variable $t = z$, we denote by $L_{C\setminus p}G \subseteq LG$ the subgroup with A–valued points $G(A \otimes_k \mathcal{O}_{C\setminus p}) \subseteq G(A((t)))$ for any k–algebra A. Consider the stack quotient $L_{C\setminus p}G\backslash \mathrm{Gr}_G$. The map $\mathrm{glue}_{p,z}$ descends to an equivalence

$$L_{C\setminus p}G\backslash \mathrm{Gr}_G \xrightarrow{\sim} \mathcal{M}_G$$

because the action of $L_{C\setminus p}G$ on Gr_G corresponds to changing trivialisations over $C \setminus \{p\}$; cf. for example [23, Theorem 1.3] or [13, Corollary 16].
More generally, consider the conjugate

$$L^\delta_{C\setminus p}G := t^{-\delta} \cdot L_{C\setminus p}G \cdot t^\delta \subseteq L\widehat{G},$$

which is actually contained in LG since LG is normal in $L\widehat{G}$. Using Lemma 4.2.2, we see that the map $\mathrm{glue}_{p,z,\delta}$ descends to an equivalence

$$L^{\delta}_{C\setminus p}G\backslash \mathrm{Gr}_G \xrightarrow{\sim} \mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)},$$

because the action of $L^{\delta}_{C\setminus p}G$ on Gr_G again corresponds to changing trivialisations over $C \setminus \{p\}$.

Let S be a scheme of finite type over k. Each line bundle on $S \times \mathcal{M}_{\widehat{G},L}$ with trivial pullback to $S \times \mathrm{Gr}_G$ comes from a character $(L^{\delta}_{C\setminus p}G)_S \longrightarrow (\mathbb{G}_m)_S$, since the map (3) is bijective. But $L^{\delta}_{C\setminus p}G$ is isomorphic to $L_{C\setminus p}G$, and every character $(L_{C\setminus p}G)_S \longrightarrow (\mathbb{G}_m)_S$ is trivial according to [13, p. 66f.]. This already shows that the morphism of Picard functors $\mathrm{glue}^*_{p,z,\delta}$ is injective.

The action of LG on Gr_G induces the trivial action on $\underline{\mathrm{Pic}}(\mathrm{Gr}_G) \cong \mathbb{Z}$, for example because it preserves ampleness, or alternatively because LG is connected. Let a line bundle $\mathcal{L}$ on Gr_G be given. We denote by $\mathrm{Mum}_{LG}(\mathcal{L})$ the Mumford group. So $\mathrm{Mum}_{LG}(\mathcal{L})$ is the functor from schemes of finite type over k to groups that sends S to the group of pairs (f, g) consisting of an element $f \in LG(S)$ and an isomorphism $g : f^*\mathcal{L}_S \xrightarrow{\sim} \mathcal{L}_S$ of line bundles on $\mathrm{Gr}_G \times S$. If $f = 1$, then $g \in \mathbb{G}_m(S)$ due to the bijectivity of (3), while for arbitrary $f \in LG(S)$, the line bundles $\mathcal{L}_S$ and $f^*\mathcal{L}_S$ have the same image in $\underline{\mathrm{Pic}}(\mathrm{Gr}_G)(S)$, implying that $\mathcal{L}_S$ and $f^*\mathcal{L}_S$ are Zariski–locally in S isomorphic. Consequently, we have a short exact sequence of sheaves in the Zariski topology

$$1 \longrightarrow \mathbb{G}_m \longrightarrow \mathrm{Mum}_{LG}(\mathcal{L}) \xrightarrow{q} LG \longrightarrow 1\,. \tag{6}$$

This central extension splits over $L^+G \subseteq LG$, because the restricted action of L^+G on Gr_G has a fixed point. We have to show that it also splits over $L^{\delta}_{C\setminus p}G \subseteq LG$.

Note that $L^{\delta}_{C\setminus p}G = \gamma(L_{C\setminus p}G)$ for the automorphism γ of LG given by conjugation with t^{δ}. Hence it is equivalent to show that the central extension

$$1 \longrightarrow \mathbb{G}_m \longrightarrow \mathrm{Mum}_{LG}(\mathcal{L}) \xrightarrow{\gamma^{-1}\circ q} LG \longrightarrow 1 \tag{7}$$

splits over $L_{C\setminus p}G$. We know already that it splits over $\gamma^{-1}(L^+G)$, in particular over $L^{\geq n}G$ for some $n \geq 1$. Thus it also splits over L^+G, due to Lemma 4.1.2. Hence it comes from a line bundle on $LG/L^+G = \mathrm{Gr}_G$ (whose associated $\mathbb{G}_m$–bundle has total space $\mathrm{Mum}_{LG}(\mathcal{L})/L^+G$, where L^+G acts from the right via the splitting). According to Theorem 4.2.1(ii), this line bundle admits a $L_{C\setminus p}G$–linearisation, and hence the extension (7) splits indeed over $L_{C\setminus p}G$.

Thus the extension (6) splits over $L^{\delta}_{C\setminus p}G$, so $\mathcal{L}$ admits an $L^{\delta}_{C\setminus p}G$–linearisation and consequently descends to $\mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)}$. This proves that $\mathrm{glue}^*_{p,z,\delta}$ is surjective as a homomorphism of Picard groups. Hence it is also surjective as a morphism of Picard functors, because $\underline{\mathrm{Pic}}(\mathrm{Gr}_G) \cong \mathbb{Z}$ is discrete by Theorem 4.2.1(i). $\square$

Remark 4.2.4. Put $G^{\mathrm{ad}} := G/Z$, where $Z \subseteq G$ denotes the center. Given a representation $\rho : G^{\mathrm{ad}} \longrightarrow \mathrm{SL}(V)$, we denote its compositions with the canonical epimorphisms $G \twoheadrightarrow G^{\mathrm{ad}}$ and $\widehat{G} \twoheadrightarrow G^{\mathrm{ad}}$ also by ρ. Then the diagram

$$\begin{array}{ccc}
\underline{\mathrm{Pic}}(\mathcal{M}_{\mathrm{SL}(V)}) & \xrightarrow{\mathrm{glue}_{p,z}^*} & \underline{\mathrm{Pic}}(\mathrm{Gr}_{\mathrm{SL}(V)}) \\
\Big\downarrow{\scriptstyle \rho^*} & & \Big\downarrow{\scriptstyle \rho^*} \\
\underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) & \xrightarrow{(t_\xi \circ \mathrm{glue}_{p,z,\delta})^*} & \underline{\mathrm{Pic}}(\mathrm{Gr}_G)
\end{array}$$

commutes.

Proof. Let $t^{\rho\circ\delta} \in L\,\mathrm{SL}(V)$ denote the image of the canonical loop $t \in L\mathbb{G}_m$ under the composition $\rho \circ \delta : \mathbb{G}_m \longrightarrow \mathrm{SL}(V)$. Then the left part of the diagram

$$\begin{array}{ccccccc}
 & & \mathrm{Gr}_G & \xrightarrow{\mathrm{glue}_{p,z,\delta}} & \mathcal{M}_{\widehat{G},\mathcal{O}_C(dp)} & \xrightarrow{t_\xi} & \mathcal{M}_{\widehat{G},L} \\
 & \swarrow{\scriptstyle \rho_*} & \Big\downarrow{\scriptstyle t^\delta\cdot_} & & \Big\downarrow & & \Big\downarrow \\
\mathrm{Gr}_{\mathrm{SL}(V)} & & \mathrm{Gr}_{\widehat{G}} & \xrightarrow{\mathrm{glue}_{p,z}} & \mathcal{M}_{\widehat{G}} & \xrightarrow{t_\xi} & \mathcal{M}_{\widehat{G}} \\
 & \searrow{\scriptstyle t^{\rho\circ\delta}\cdot_} & \Big\downarrow{\scriptstyle \rho_*} & & \Big\downarrow{\scriptstyle \rho_*} & & \Big\downarrow{\scriptstyle \rho_*} \\
 & & \mathrm{Gr}_{\mathrm{SL}(V)} & \xrightarrow{\mathrm{glue}_{p,z}} & \mathcal{M}_{\mathrm{SL}(V)} & = & \mathcal{M}_{\mathrm{SL}(V)}
\end{array}$$

commutes. The four remaining squares are 2–commutative by construction of the 1–morphisms $\mathrm{glue}_{p,z,\delta}$, $\mathrm{glue}_{p,z}$ and t_ξ. Applying $\underline{\mathrm{Pic}}$ to the exterior pentagon yields the required commutative square, as $L\,\mathrm{SL}(V)$ acts trivially on $\underline{\mathrm{Pic}}(\mathrm{Gr}_{\mathrm{SL}(V)})$. □

4.3. Néron–Severi groups $\mathrm{NS}(\mathcal{M}_G)$ for simply connected G. Let G be a reductive group over k; later in this subsection, we will assume that G is simply connected. Choose a maximal torus $T_G \subseteq G$, and let

$$\mathrm{Hom}(\Lambda_{T_G} \otimes \Lambda_{T_G}, \mathbb{Z})^W \tag{8}$$

denote the abelian group of bilinear forms $b : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathbb{Z}$ that are invariant under the Weyl group $W = W_G$ of (G, T_G).

Up to a *canonical* isomorphism, the group (8) does not depend on the choice of T_G. More precisely, let $T'_G \subseteq G$ be another maximal torus; then the conjugation $\gamma_g : G \longrightarrow G$ with some $g \in G(k)$ provides an isomorphism from T_G to T'_G, and the induced isomorphism from $\mathrm{Hom}(\Lambda_{T'_G} \otimes \Lambda_{T'_G}, \mathbb{Z})^W$ to $\mathrm{Hom}(\Lambda_{T_G} \otimes \Lambda_{T_G}, \mathbb{Z})^W$ does not depend on the choice of g.

The group (8) is also functorial in G. More precisely, let $\varphi : G \longrightarrow H$ be a homomorphism of reductive groups over k. Choose a maximal torus $T_H \subseteq H$ containing $\varphi(T_G)$.

Lemma 4.3.1. *Let $T'_G \subseteq G$ be another maximal torus, and let $T'_H \subseteq H$ be a maximal torus containing $\varphi(T'_G)$. For every $g \in G(k)$ with $T'_G = \gamma_g(T_G)$, there* *is an $h \in H(k)$ with $T'_H = \gamma_h(T_H)$ such that the following diagram commutes:*

$$\begin{CD}
T_G @>{\gamma_g}>> T'_G \\
@V{\varphi}VV @VV{\varphi}V \\
T_H @>{\gamma_h}>> T'_H
\end{CD}$$

Proof. The diagram

$$\begin{CD}
T_G @= T_G @>{\gamma_g}>> T'_G \\
@V{\varphi}VV @V{\varphi}VV @VV{\varphi}V \\
T_H @>>> \gamma^{-1}_{\varphi(g)}(T'_H) @>{\gamma_{\varphi(g)}}>> T'_H
\end{CD}$$

allows us to assume $T'_G = T_G$ and $g = 1$ without loss of generality. Then T_H and T'_H are maximal tori in the centraliser of $\varphi(T_G)$, which is reductive according to [17, 26.2. Corollary A]. Thus $T'_H = \gamma_h(T_H)$ for an appropriate k–point h of this centraliser, and $\gamma_h \circ \varphi = \varphi$ on T_G by definition of the centraliser. $\square$

Applying the lemma with $T'_G = T_G$ and $T'_H = T_H$, we see that the pullback along $\varphi_* : \Lambda_{T_G} \longrightarrow \Lambda_{T_H}$ of a W_H–invariant form $\Lambda_{T_H} \otimes \Lambda_{T_H} \longrightarrow \mathbb{Z}$ is W_G–invariant, so we get an induced map

$$\varphi^* : \mathrm{Hom}(\Lambda_{T_H} \otimes \Lambda_{T_H}, \mathbb{Z})^{W_H} \longrightarrow \mathrm{Hom}(\Lambda_{T_G} \otimes \Lambda_{T_G}, \mathbb{Z})^{W_G} \tag{9}$$

which does not depend on the choice of T_G and T_H by the above lemma again. *For the rest of this subsection, we assume that G and H are simply connected.*

Definition 4.3.2. i) The *Néron–Severi group* $\mathrm{NS}(\mathcal{M}_G)$ is the subgroup

$$\mathrm{NS}(\mathcal{M}_G) \subseteq \mathrm{Hom}(\Lambda_{T_G} \otimes \Lambda_{T_G}, \mathbb{Z})^W$$

of symmetric forms $b : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathbb{Z}$ with $b(\lambda \otimes \lambda) \in 2\mathbb{Z}$ for all $\lambda \in \Lambda_{T_G}$.

ii) Given a homomorphism $\varphi : G \longrightarrow H$, we denote by

$$\varphi^* : \mathrm{NS}(\mathcal{M}_H) \longrightarrow \mathrm{NS}(\mathcal{M}_G)$$

the restriction of the induced map φ^* in (9).

Remarks 4.3.3. i) If $G = G_1 \times G_2$ for simply connected groups G_1 and G_2, then

$$\mathrm{NS}(\mathcal{M}_G) = \mathrm{NS}(\mathcal{M}_{G_1}) \oplus \mathrm{NS}(\mathcal{M}_{G_2}),$$

since each element of $\mathrm{Hom}(\Lambda_{T_G} \otimes \Lambda_{T_G}, \mathbb{Z})^{W_G}$ vanishes on $\Lambda_{T_{G_1}} \otimes \Lambda_{T_{G_2}} + \Lambda_{T_{G_2}} \otimes \Lambda_{T_{G_1}}$.

ii) If on the other hand G is almost simple, then

$$\mathrm{NS}(\mathcal{M}_G) = \mathbb{Z} \cdot b_G$$

where the *basic inner product* b_G is the unique element of $\mathrm{NS}(\mathcal{M}_G)$ that satisfies $b_G(\alpha^\vee, \alpha^\vee) = 2$ for all short coroots $\alpha^\vee \in \Lambda_{T_G}$ of G.

iii) Let G and H be almost simple. The *Dynkin index* $d_\varphi \in \mathbb{Z}$ of a homomorphism $\varphi : G \longrightarrow H$ is defined by $\varphi^*(b_H) = d_\varphi \cdot b_G$, cf. [11, §2]. If φ is nontrivial, then $d_\varphi > 0$, since b_G and b_H are positive definite.

Let $Z \subseteq G$ be the center. Then $G^{\mathrm{ad}} := G/Z$ contains $T_{G^{\mathrm{ad}}} := T_G/Z$ as a maximal torus, with cocharacter lattice $\Lambda_{T_{G^{\mathrm{ad}}}} \subseteq \Lambda_{T_G} \otimes \mathbb{Q}$.
We say that a homomorphism $l : \Lambda \longrightarrow \Lambda'$ between finitely generated free abelian groups Λ and Λ' is *integral* on a subgroup $\widetilde{\Lambda} \subseteq \Lambda \otimes \mathbb{Q}$ if its restriction to $\Lambda \cap \widetilde{\Lambda}$ admits a linear extension $\widetilde{l} : \widetilde{\Lambda} \longrightarrow \Lambda'$. By abuse of language, we will not distinguish between l and its unique linear extension $\widetilde{l}$.

Lemma 4.3.4. *Every element $b : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathbb{Z}$ of $\mathrm{NS}(\mathcal{M}_G)$ is integral on $\Lambda_{T_{G^{ad}}} \otimes \Lambda_{T_G}$ and on $\Lambda_{T_G} \otimes \Lambda_{T_{G^{ad}}}$.*

Proof. Let $\alpha : \Lambda_{T_G} \otimes \mathbb{Q} \longrightarrow \mathbb{Q}$ be a root of G, with corresponding coroot $\alpha^\vee \in \Lambda_{T_G}$. Lemme 2 in [5, Chapitre VI, §1] implies the formula

$$b(\lambda \otimes \alpha^\vee) = \alpha(\lambda) \cdot b(\alpha^\vee \otimes \alpha^\vee)/2$$

for all $\lambda \in \Lambda_{T_G}$. Thus $b(\_ \otimes \alpha^\vee) : \Lambda_{T_G} \longrightarrow \mathbb{Z}$ is an integer multiple of α; hence it is integral on $\Lambda_{T_{G^{\mathrm{ad}}}}$, the largest subgroup of $\Lambda_{T_G} \otimes \mathbb{Q}$ on which all roots are integral. But the coroots $\alpha^\vee$ generate Λ_{T_G}, as G is simply connected. □

Now let $\iota_G : T_G \hookrightarrow G$ denote the inclusion of the chosen maximal torus.

Definition 4.3.5. Given $\delta \in \Lambda_{T_{G^{\mathrm{ad}}}}$, the homomorphism

$$(\iota_G)^{\mathrm{NS},\delta} : \mathrm{NS}(\mathcal{M}_G) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_G})$$

sends $b : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathbb{Z}$ to

$$b(-\delta \otimes \_) : \Lambda_{T_G} \longrightarrow \mathbb{Z} \qquad \text{and} \qquad \mathrm{id}_{J_C} \cdot b : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathrm{End}\, J_C.$$

This map $(\iota_G)^{\mathrm{NS},\delta}$ is injective if $g_C \geq 1$, because all multiples of id_{J_C} are then nonzero in $\mathrm{End}\, J_C$. If $g_C = 0$, then $\mathrm{End}\, J_C = 0$, but we still have the following

Lemma 4.3.6. *Every coset $d \in \Lambda_{T_{G^{ad}}}/\Lambda_{T_G} = \pi_1(G^{ad})$ admits a lift $\delta \in \Lambda_{T_{G^{ad}}}$ such that the map $(\iota_G)^{\mathrm{NS},\delta} : \mathrm{NS}(\mathcal{M}_G) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_G})$ is injective.*

Proof. Using Remark 4.3.3, we may assume that G is almost simple. In this case, $(\iota_G)^{\mathrm{NS},\delta}$ is injective whenever $\delta \neq 0$, because $\mathrm{NS}(\mathcal{M}_G)$ is cyclic and its generator $b_G : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathbb{Z}$ is as a bilinear form nondegenerate. □

Remark 4.3.7. Given $\varphi : G \longrightarrow H$, let $\iota_H : T_H \hookrightarrow H$ be a maximal torus with $\varphi(T_G) \subseteq T_H$. If $\delta \in \Lambda_{T_G}$, or if more generally $\delta \in \Lambda_{T_{G^{\mathrm{ad}}}}$ is mapped to $\Lambda_{H^{\mathrm{ad}}}$ by $\varphi_* : \Lambda_{T_G} \otimes \mathbb{Q} \longrightarrow \Lambda_{T_H} \otimes \mathbb{Q}$, then the following diagram commutes:

$$\begin{array}{ccc}
\mathrm{NS}(\mathcal{M}_H) & \xrightarrow{(\iota_H)^{\mathrm{NS},\varphi_*\delta}} & \mathrm{NS}(\mathcal{M}_{T_H}) \\
\Big\downarrow \varphi_* & & \Big\downarrow \varphi_* \\
\mathrm{NS}(\mathcal{M}_G) & \xrightarrow{(\iota_G)^{\mathrm{NS},\delta}} & \mathrm{NS}(\mathcal{M}_{T_G})
\end{array}$$

4.4. THE PULLBACK TO TORUS BUNDLES. Let $\mathcal{L}^{\det} = \mathcal{L}_n^{\det}$ be determinant of cohomology line bundle [18] on $\mathcal{M}_{\mathrm{GL}_n}$, whose fibre at a vector bundle E on C is $\det \mathrm{H}^*(E) = \det \mathrm{H}^0(E) \otimes \det \mathrm{H}^1(E)^{\mathrm{dual}}$.

LEMMA 4.4.1. *Let ξ be a line bundle of degree d on C. Then the composition*

$$\mathrm{Pic}(\mathcal{M}_{\mathbb{G}_m}) \xrightarrow{t_\xi^*} \mathrm{Pic}(\mathcal{M}_{\mathbb{G}_m}^0) \xrightarrow{c_{\mathbb{G}_m}} \mathrm{NS}(\mathcal{M}_{\mathbb{G}_m}) = \mathbb{Z} \oplus \mathrm{End}_{J_C}$$

maps $\mathcal{L}^{\det}$ to $1 - g_C + d \in \mathbb{Z}$ and $-\mathrm{id}_{J_C} \in \mathrm{End}_{J_C}$.

Proof. For any line bundle L on C and any point $p \in C(k)$, we have a canonical exact sequence

$$0 \longrightarrow L(-p) \longrightarrow L \longrightarrow L_p \longrightarrow 0$$

of coherent sheaves on C. Varying L and taking the determinant of cohomology, we see that the two line bundles $\mathcal{L}^{\det}$ and $t_{\mathcal{O}(-p)}^*\mathcal{L}^{\det}$ on $\mathcal{M}_{\mathbb{G}_m}^0$ have the same image in the second summand $\mathrm{End}\, J_C$ of $\mathrm{NS}(\mathcal{M}_{\mathbb{G}_m})$. Thus the image of $t_\xi^*\mathcal{L}^{\det}$ in $\mathrm{End}\, J_C$ does not depend on ξ; this image is $-\mathrm{id}_{J_C}$ because the principal polarisation $\phi_\Theta : J_C \longrightarrow J_C^\vee$ is essentially given by the dual of the line bundle $\mathcal{L}^{\det}$.
The weight of $t_\xi^*\mathcal{L}^{\det}$ at a line bundle L of degree 0 on C is the Euler characteristic of $L \otimes \xi$, which is indeed $1 - g_C + d$ by Riemann–Roch theorem. □

Let $\iota : T_{\mathrm{SL}_n} \hookrightarrow \mathrm{SL}_n$ be the inclusion of the maximal torus $T_{\mathrm{SL}_n} := \mathbb{G}_m^n \cap \mathrm{SL}_n$, where $\mathbb{G}_m^n \subseteq \mathrm{GL}_n$ as diagonal matrices. Then the cocharacter lattice $\Lambda_{T_{\mathrm{SL}_n}}$ is the group of all $d = (d_1, \ldots, d_n) \in \mathbb{Z}^n$ with $d_1 + \cdots + d_n = 0$. The basic inner product $b_{\mathrm{SL}_n} : \Lambda_{T_{\mathrm{SL}_n}} \otimes \Lambda_{T_{\mathrm{SL}_n}} \longrightarrow \mathbb{Z}$ is the restriction of the standard scalar product on $\mathbb{Z}^n$.

COROLLARY 4.4.2. *Let ξ be a principal T_{SL_n}–bundle of degree $d \in \Lambda_{T_{\mathrm{SL}_n}}$ on C. Then the composition*

$$\mathrm{Pic}(\mathcal{M}_{\mathrm{SL}_n}) \xrightarrow{\iota^*} \mathrm{Pic}(\mathcal{M}_{T_{\mathrm{SL}_n}}) \xrightarrow{t_\xi^*} \mathrm{Pic}(\mathcal{M}_{T_{\mathrm{SL}_n}}^0) \xrightarrow{c_{T_{\mathrm{SL}_n}}} \mathrm{NS}(\mathcal{M}_{T_{\mathrm{SL}_n}})$$

maps $\mathcal{L}^{\det}$ to $b_{\mathrm{SL}_n}(d \otimes \_) : \Lambda_{T_{\mathrm{SL}_n}} \longrightarrow \mathbb{Z}$ and $-\mathrm{id}_{J_C} \cdot b_{\mathrm{SL}_n} : \Lambda_{T_{\mathrm{SL}_n}} \otimes \Lambda_{T_{\mathrm{SL}_n}} \longrightarrow \mathrm{End}\, J_C$.

Proof. Since the determinant of cohomology takes direct sums to tensor products, the pullback of $\mathcal{L}_n^{\det}$ to $\mathcal{M}_{\mathbb{G}_m^n}$ is isomorphic to $\mathrm{pr}_1^* \mathcal{L}_1^{\det} \otimes \cdots \otimes \mathrm{pr}_n^* \mathcal{L}_1^{\det}$, where $\mathrm{pr}_\nu : \mathbb{G}_m^n \twoheadrightarrow \mathbb{G}_m$ is the projection onto the νth factor. Now use the previous lemma to compute the image of $\mathcal{L}_n^{\det}$ in $\mathrm{NS}(\mathcal{M}_{\mathbb{G}_m^n})$ and then restrict to $\mathrm{NS}(\mathcal{M}_{T_{\mathrm{SL}_n}})$. □

COROLLARY 4.4.3. *If $\rho : \mathrm{SL}_2 \longrightarrow \mathrm{SL}(V)$ has Dynkin index d_ρ, then the pullback $\rho^* : \mathrm{Pic}(\mathcal{M}_{\mathrm{SL}(V)}) \longrightarrow \mathrm{Pic}(\mathcal{M}_{\mathrm{SL}_2})$ maps $\mathcal{L}^{\det}$ to $(\mathcal{L}_2^{\det})^{\otimes d_\rho}$.*

Proof. Let $\iota : T_{\mathrm{SL}(V)} \hookrightarrow \mathrm{SL}(V)$ be the inclusion of a maximal torus that contains the image of the standard torus $T_{\mathrm{SL}_2} \hookrightarrow \mathrm{SL}_2$. The diagram

$$\begin{array}{ccccccc}
\mathrm{Pic}(\mathcal{M}_{\mathrm{SL}(V)}) & \xrightarrow{\iota^*} & \mathrm{Pic}(\mathcal{M}_{T_{\mathrm{SL}(V)}}) & \xrightarrow{t^*_{\rho_*(\xi)}} & \mathrm{Pic}(\mathcal{M}^0_{T_{\mathrm{SL}(V)}}) & \xrightarrow{c_{T_{\mathrm{SL}(V)}}} & \mathrm{NS}(\mathcal{M}_{T_{\mathrm{SL}(V)}}) \\
\downarrow{\scriptstyle \rho^*} & & \downarrow{\scriptstyle \rho^*} & & \downarrow{\scriptstyle \rho^*} & & \downarrow{\scriptstyle \rho^*} \\
\mathrm{Pic}(\mathcal{M}_{\mathrm{SL}_2}) & \xrightarrow{\iota^*} & \mathrm{Pic}(\mathcal{M}_{T_{\mathrm{SL}_2}}) & \xrightarrow{t^*_{\xi}} & \mathrm{Pic}(\mathcal{M}^0_{T_{\mathrm{SL}_2}}) & \xrightarrow{c_{T_{\mathrm{SL}_2}}} & \mathrm{NS}(\mathcal{M}_{T_{\mathrm{SL}_2}})
\end{array}$$

commutes for each principal T_{SL_2}–bundle ξ on C. We choose ξ in such a way that $\deg(\xi) \in \Lambda_{T_{\mathrm{SL}_2}} \cong \mathbb{Z}$ is nonzero if $g_C = 0$. Then the composition

$$c_{T_{\mathrm{SL}_2}} \circ t^*_\xi \circ \iota^* : \mathrm{Pic}(\mathcal{M}_{\mathrm{SL}_2}) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_{\mathrm{SL}_2}})$$

of the lower row is injective according to Theorem 4.2.1 and Corollary 4.4.2. The latter moreover implies that the two elements $\rho^*(\mathcal{L}^{\det})$ and $(\mathcal{L}_2^{\det})^{\otimes d_\rho}$ in $\mathrm{Pic}(\mathcal{M}_{\mathrm{SL}_2})$ have the same image in $\mathrm{NS}(\mathcal{M}_{T_{\mathrm{SL}_2}})$. □

Now suppose that the reductive group G is simply connected and almost simple. We denote by $\mathcal{O}_{\mathrm{Gr}_G}(1)$ the unique generator of $\mathrm{Pic}(\mathrm{Gr}_G)$ that is ample on every closed subscheme, and by $\mathcal{O}_{\mathrm{Gr}_G}(n)$ its nth tensor power for $n \in \mathbb{Z}$.
Over $k = \mathbb{C}$, the following is proved by a different method in section 5 of [20].

Proposition 4.4.4 (Kumar-Narasimhan-Ramanathan). *If $\rho : G \longrightarrow \mathrm{SL}(V)$ has Dynkin index d_ρ, then $\rho^* : \mathrm{Pic}(\mathrm{Gr}_{\mathrm{SL}(V)}) \longrightarrow \mathrm{Pic}(\mathrm{Gr}_G)$ maps $\mathcal{O}(1)$ to $\mathcal{O}_{\mathrm{Gr}_G}(d_\rho)$.*

Proof. Let $\varphi : \mathrm{SL}_2 \longrightarrow G$ be given by a short coroot. Then $d_\varphi = 1$ by definition, and [13] implies that $\varphi^* : \mathrm{Pic}(\mathrm{Gr}_G) \longrightarrow \mathrm{Pic}(\mathrm{Gr}_{\mathrm{SL}_2})$ maps $\mathcal{O}(1)$ to $\mathcal{O}(1)$, for example because $\varphi^* : \mathrm{Pic}(\mathcal{M}_G) \longrightarrow \mathrm{Pic}(\mathcal{M}_{\mathrm{SL}_2})$ preserves central charges according to their definition [13, p. 59]. Hence it suffices to prove the claim for $\rho \circ \varphi$ instead of ρ. This case follows from Corollary 4.4.3, since $\mathrm{glue}^*_{p,z}(\mathcal{L}^{\det}_n) \cong \mathcal{O}_{\mathrm{Gr}_{\mathrm{SL}_n}}(-1)$. □

As in Subsection 4.2, we assume given an exact sequence of reductive groups

$$1 \longrightarrow G \longrightarrow \widehat{G} \xrightarrow{\mathrm{dt}} \mathbb{G}_m \longrightarrow 1$$

with G simply connected, and a line bundle L on C.

Corollary 4.4.5. *Suppose that G is almost simple. Then the isomorphism*

$$(t_\xi \circ \mathrm{glue}_{p,z,\delta})^* : \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) \xrightarrow{\sim} \underline{\mathrm{Pic}}(\mathrm{Gr}_G)$$

constructed in Subsection 4.2 does not depend on the choice of p, z, ξ or δ.

We say that a line bundle on $\mathcal{M}_{\widehat{G},L}$ has *central charge* $n \in \mathbb{Z}$ if this isomorphism maps it to $\mathcal{O}_{\mathrm{Gr}_G}(n)$; this is consistent with the standard central charge of line bundles on $\mathcal{M}_G$, as defined for example in [13].

Proof. If $\rho : G \longrightarrow \mathrm{SL}(V)$ is a nontrivial representation, then $d_\rho > 0$, as explained in Remark 4.3.3(iii). Using Proposition 4.4.4, this implies that

$$\rho^* : \mathrm{Pic}(\mathrm{Gr}_{\mathrm{SL}(V)}) \longrightarrow \mathrm{Pic}(\mathrm{Gr}_G)$$

is injective. Due to Remark 4.2.4, it thus suffices to check that

$$\mathrm{glue}_{p,z}^* : \underline{\mathrm{Pic}}(\mathcal{M}_{\mathrm{SL}(V)}) \xrightarrow{\sim} \underline{\mathrm{Pic}}(\mathrm{Gr}_{\mathrm{SL}(V)})$$

does not depend on p or z. This is clear, since it maps $\mathcal{L}^{\det}$ to $\mathcal{O}_{\mathrm{Gr}_{\mathrm{SL}(V)}}(-1)$. □

The chosen maximal torus $\iota_G : T_G \hookrightarrow G$ induces maximal tori $\iota_{\widehat{G}} : T_{\widehat{G}} \hookrightarrow \widehat{G}$ and $\iota_{G^{\mathrm{ad}}} : T_{G^{\mathrm{ad}}} \hookrightarrow G^{\mathrm{ad}}$ compatible with the canonical maps $G \hookrightarrow \widehat{G} \twoheadrightarrow G^{\mathrm{ad}}$. Given a principal $T_{\widehat{G}}$–bundle $\widehat{\xi}$ on C and an isomorphism $\mathrm{dt}_* \widehat{\xi} \cong L$, the composition

$$\mathcal{M}_{T_G}^0 \xrightarrow{t_{\widehat{\xi}}} \mathcal{M}_{T_{\widehat{G}}} \xrightarrow{(\iota_{\widehat{G}})_*} \mathcal{M}_{\widehat{G}}$$

factors naturally through a 1–morphism

$$\iota_{\widehat{\xi}} : \mathcal{M}_{T_G}^0 \longrightarrow \mathcal{M}_{\widehat{G},L}. \tag{10}$$

Remark 4.4.6. Given a representation $\rho : G^{\mathrm{ad}} \longrightarrow \mathrm{SL}(V)$, let $\iota : T_{\mathrm{SL}(V)} \hookrightarrow \mathrm{SL}(V)$ be a maximal torus containing $\rho(T_{G^{\mathrm{ad}}})$. Then the diagram

$$\begin{array}{ccccc}
\mathcal{M}_{T_G}^0 & & \xrightarrow{\quad\iota_{\widehat{\xi}}\quad} & & \mathcal{M}_{\widehat{G},L} \\
\downarrow{\scriptstyle \rho_*} & & & & \downarrow{\scriptstyle \rho_*} \\
\mathcal{M}_{T_{\mathrm{SL}(V)}}^0 & \xrightarrow{t_{\rho_*\widehat{\xi}}} & \mathcal{M}_{T_{\mathrm{SL}(V)}} & \xrightarrow{\iota_*} & \mathcal{M}_{\mathrm{SL}(V)}
\end{array}$$

is 2–commutative, by construction of $\iota_{\widehat{\xi}}$.

Proposition 4.4.7. i) $\Gamma(\mathcal{M}_{\widehat{G},L}, \mathcal{O}_{\mathcal{M}_{\widehat{G},L}}) = k$.

ii) *There is a canonical isomorphism*

$$c_G : \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) \xrightarrow{\sim} \mathrm{NS}(\mathcal{M}_G).$$

iii) *For all choices of $\iota_G : T_G \hookrightarrow G$ and of $\widehat{\xi}$, the diagram*

$$\begin{array}{ccc}
\underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) & \xrightarrow{\quad\iota_{\widehat{\xi}}^*\quad} & \underline{\mathrm{Pic}}(\mathcal{M}_{T_G}^0) \\
\downarrow{\scriptstyle c_G} & & \downarrow{\scriptstyle c_{T_G}} \\
\mathrm{NS}(\mathcal{M}_G) & \xrightarrow{(\iota_G)^{\mathrm{NS},\bar{\delta}}} & \mathrm{NS}(\mathcal{M}_{T_G})
\end{array}$$

commutes; here $\bar{\delta} \in \Lambda_{T_{G^{ad}}}$ denotes the image of $\widehat{\delta} := \deg \widehat{\xi} \in \Lambda_{T_{\widehat{G}}}$.

Proof. We start with the special case that G is almost simple. Here part (i) of the proposition is just equation (5) from Subsection 4.2.
We let c_G send the line bundle of central charge 1 to the basic inner product $b_G \in \mathrm{NS}(\mathcal{M}_G)$. Due to Theorem 4.2.1(i), Proposition 4.2.3, Corollary 4.4.5

and Remark 4.3.3(ii), this defines a canonical isomorphism, and hence proves (ii).
To see that the diagram in (iii) then commutes, we choose a nontrivial representation $\rho : G^{\mathrm{ad}} \longrightarrow \mathrm{SL}(V)$. We note the functorialities, with respect to ρ, according to Remark 4.4.6, Remark 4.2.4, Proposition 4.4.4, Remark 4.3.7 and Remark 3.2.3. In view of these, comparing Corollary 4.4.2 and Definition 4.3.5 shows that the two images of $\rho^*\mathcal{L}^{\det} \in \mathrm{Pic}(\mathcal{M}_{\widehat{G},L})$ in $\mathrm{NS}(\mathcal{M}_{T_G})$ coincide. Since the former generates a subgroup of finite index and the latter is torsionfree, the diagram in (iii) commutes.
For the general case, we use the unique decomposition

$$G = G_1 \times \cdots \times G_r$$

into simply connected and almost simple factors G_i. As $\widehat{G}$ is generated by its center and G, every normal subgroup in G is still normal in $\widehat{G}$. Let $\widehat{G}_i$ denote the quotient of $\widehat{G}$ modulo the closed normal subgroup $\prod_{j \neq i} G_j$; then

$$\begin{array}{ccccccccc} 0 & \longrightarrow & G & \longrightarrow & \widehat{G} & \longrightarrow & \mathbb{G}_m & \longrightarrow & 0 \\ & & \downarrow{\scriptstyle \mathrm{pr}_i} & & \downarrow & & \| & & \\ 0 & \longrightarrow & G_i & \longrightarrow & \widehat{G}_i & \xrightarrow{\mathrm{dt}_i} & \mathbb{G}_m & \longrightarrow & 0 \end{array}$$

is a morphism of short exact sequences. Since the resulting diagram

$$\begin{array}{ccc} \widehat{G} & \longrightarrow & \prod_i \widehat{G}_i \\ {\scriptstyle \mathrm{dt}}\downarrow & & \downarrow{\scriptstyle \prod \mathrm{dt}_i} \\ \mathbb{G}_m & \xrightarrow{\mathrm{diag}} & \mathbb{G}_m^r \end{array}$$

is cartesian, it induces an equivalence of moduli stacks

$$\mathcal{M}_{\widehat{G},L} \xrightarrow{\sim} \mathcal{M}_{\widehat{G}_1,L} \times \cdots \times \mathcal{M}_{\widehat{G}_r,L} \tag{11}$$

due to Lemma 2.2.1. We note that equation (5), Lemma 2.1.2(i), Lemma 2.1.4, Remark 4.3.3(i) and Corollary 3.2.4 ensure that various constructions are compatible with the products in (11). Therefore, the general case follows from the already treated almost simple case. □

5. The reductive case

In this section, we finally describe the Picard functor $\underline{\mathrm{Pic}}(\mathcal{M}_G^d)$ for any reductive group G over k and any $d \in \pi_1(G)$. We denote

- by $\zeta : Z^0 \hookrightarrow G$ the (reduced) identity component of the center $Z \subseteq G$, and
- by $\pi : \widetilde{G} \longrightarrow G$ the universal cover of $G' := [G, G] \subseteq G$.

Our strategy is to descend along the central isogeny

$$\zeta \cdot \pi : Z^0 \times \widetilde{G} \longrightarrow G,$$

applying the previous two sections to Z^0 and to $\widetilde{G}$, respectively. The 1–morphism of moduli stacks given by such a central isogeny is a torsor under a group stack; Subsection 5.1 explains descent of line bundles along such torsors, generalising the method introduced by Laszlo [22] for quotients of SL_n. In Subsection 5.2, we define combinatorially what will be the discrete torsionfree part of $\underline{\mathrm{Pic}}(\mathcal{M}_G^d)$; finally, these Picard functors and their functoriality in G are described in Subsection 5.3.
The following notation is used throughout this section. The reductive group G yields semisimple groups and central isogenies

$$\widetilde{G} \twoheadrightarrow G' \twoheadrightarrow \bar{G} := G/Z^0 \twoheadrightarrow G^{\mathrm{ad}} := G/Z.$$

We denote by $\bar{d} \in \pi_1(\bar{G}) \subseteq \pi_1(G^{\mathrm{ad}})$ the image of $d \in \pi_1(G)$. The choice of a maximal torus $\iota_G : T_G \hookrightarrow G$ induces maximal tori and isogenies

$$T_{\widetilde{G}} \twoheadrightarrow T_{G'} \twoheadrightarrow T_{\bar{G}} \twoheadrightarrow T_{G^{\mathrm{ad}}}.$$

Their cocharacter lattices are hence subgroups of finite index

$$\Lambda_{T_{\widetilde{G}}} \hookrightarrow \Lambda_{T_{G'}} \hookrightarrow \Lambda_{T_{\bar{G}}} \hookrightarrow \Lambda_{T_{G^{\mathrm{ad}}}}.$$

The central isogeny $\zeta \cdot \pi$ makes $\Lambda_{Z^0} \oplus \Lambda_{T_{\widetilde{G}}}$ a subgroup of finite index in Λ_{T_G}.

5.1. Torsors under a group stack. All stacks in this subsection are stacks over k, and all morphisms are over k. Following [7, 22], we recall the notion of a torsor under a group stack.
Let $\mathcal{G}$ be a group stack. We denote by 1 the unit object in $\mathcal{G}$, and by $g_1 \cdot g_2$ the image of two objects g_1 and g_2 under the multiplication 1–morphism $\mathcal{G} \times \mathcal{G} \longrightarrow \mathcal{G}$.

Definition 5.1.1. An *action* of $\mathcal{G}$ on a 1–morphism of stacks $\Phi : \mathcal{X} \longrightarrow \mathcal{Y}$ consists of a 1–morphism

$$\mathcal{G} \times \mathcal{X} \longrightarrow \mathcal{X}, \qquad (g, x) \longmapsto g \cdot x,$$

and of three 2–morphisms, which assign to each k–scheme S and each object

x in $\mathcal{X}(S)$	an isomorphism $1 \cdot x \xrightarrow{\sim} x$ in $\mathcal{X}(S)$,
(g, x) in $(\mathcal{G} \times \mathcal{X})(S)$	an isomorphism $\Phi(g \cdot x) \xrightarrow{\sim} \Phi(x)$ in $\mathcal{Y}(S)$,
(g_1, g_2, x) in $(\mathcal{G} \times \mathcal{G} \times \mathcal{X})(S)$	an isomorphism $(g_1 \cdot g_2) \cdot x \xrightarrow{\sim} g_1 \cdot (g_2 \cdot x)$ in $\mathcal{X}(S)$.

These morphisms are required to satisfy the following five compatibility conditions: the two resulting isomorphisms

$$(g \cdot 1) \cdot x \xrightarrow{\sim} g \cdot x \text{ in } \mathcal{X}(S),$$
$$(1 \cdot g) \cdot x \xrightarrow{\sim} g \cdot x \text{ in } \mathcal{X}(S),$$
$$\Phi(1 \cdot x) \xrightarrow{\sim} \Phi(x) \text{ in } \mathcal{Y}(S),$$
$$\Phi((g_1 \cdot g_2) \cdot x) \xrightarrow{\sim} \Phi(x) \text{ in } \mathcal{Y}(S),$$
$$\text{and } (g_1 \cdot g_2 \cdot g_3) \cdot x \xrightarrow{\sim} g_1 \cdot (g_2 \cdot (g_3 \cdot x)) \text{ in } \mathcal{X}(S),$$

coincide for all k–schemes S and all objects g, g_1, g_2, g_3 in $\mathcal{G}(S)$ and x in $\mathcal{X}(S)$.

Example 5.1.2. Let $\varphi : G \longrightarrow H$ be a homomorphism of linear algebraic groups over k, and let Z be a closed subgroup in the center of G with $Z \subseteq \ker(\varphi)$. Then the group stack $\mathcal{M}_Z$ acts on the 1–morphism $\varphi_* : \mathcal{M}_G \longrightarrow \mathcal{M}_H$ via the tensor product $\_ \otimes \_ : \mathcal{M}_Z \times \mathcal{M}_G \longrightarrow \mathcal{M}_G$.

From now on, we assume that the group stack $\mathcal{G}$ is algebraic.

Definition 5.1.3. A *$\mathcal{G}$–torsor* is a faithfully flat 1–morphism of algebraic stacks $\Phi : \mathcal{X} \longrightarrow \mathcal{Y}$ together with an action of $\mathcal{G}$ on Φ such that the resulting 1–morphism

$$\mathcal{G} \times \mathcal{X} \longrightarrow \mathcal{X} \times_{\mathcal{Y}} \mathcal{X}, \quad (g, x) \longmapsto (g \cdot x, x)$$

is an isomorphism.

Example 5.1.4. Suppose that $\varphi : G \twoheadrightarrow H$ is a central isogeny of reductive groups with kernel μ. For each $d \in \pi_1(G)$, the 1–morphism

$$\varphi_* : \mathcal{M}_G^d \longrightarrow \mathcal{M}_H^e \qquad e := \varphi_*(d) \in \pi_1(H) \tag{12}$$

is a torsor under the group stack $\mathcal{M}_\mu$, for the action described in example 5.1.2.

Proof. The 1–morphism φ_* is faithfully flat by Lemma 2.2.2. The 1–morphism

$$\mathcal{M}_\mu \times \mathcal{M}_G \longrightarrow \mathcal{M}_G \times_{\mathcal{M}_H} \mathcal{M}_G, \quad (L, E) \longmapsto (L \otimes E, E)$$

is an isomorphism due to Lemma 2.2.1. Since $\varphi_* : \pi_1(G) \longrightarrow \pi_1(H)$ is injective, $\mathcal{M}_G^d \subseteq \mathcal{M}_G$ is the inverse image of $\mathcal{M}_H^e \subseteq \mathcal{M}_H$ under φ_*; hence the restriction

$$\mathcal{M}_\mu \times \mathcal{M}_G^d \longrightarrow \mathcal{M}_G^d \times_{\mathcal{M}_H^e} \mathcal{M}_G^d$$

is an isomorphism as well. □

Definition 5.1.5. Let $\Phi_\nu : \mathcal{X}_\nu \longrightarrow \mathcal{Y}_\nu$ be a $\mathcal{G}$–torsor for $\nu = 1, 2$. A *morphism of $\mathcal{G}$–torsors* from Φ_1 to Φ_2 consists of two 1–morphisms

$$A : \mathcal{X}_1 \longrightarrow \mathcal{X}_2 \qquad \text{and} \qquad B : \mathcal{Y}_1 \longrightarrow \mathcal{Y}_2$$

and of two 2–morphisms, which assign to each k–scheme S and each object

x in $\mathcal{X}_1(S)$	an isomorphism $\Phi_2 A(x) \xrightarrow{\sim} B\Phi_1(x)$ in $\mathcal{Y}_2(S)$,
(g, x) in $(\mathcal{G} \times \mathcal{X}_1)(S)$	an isomorphism $A(g \cdot x) \xrightarrow{\sim} g \cdot A(x)$ in $\mathcal{X}_2(S)$.

These morphisms are required to satisfy the following three compatibility conditions: the two resulting isomorphisms

$$A(1 \cdot x) \xrightarrow{\sim} A(x) \text{ in } \mathcal{X}_2(S),$$
$$\Phi_2 A(g \cdot x) \xrightarrow{\sim} B\Phi_1(x) \text{ in } \mathcal{Y}_2(S)$$
$$\text{and } A((g_1 \cdot g_2) \cdot x) \xrightarrow{\sim} g_1 \cdot (g_2 \cdot A(x)) \text{ in } \mathcal{X}_2(S)$$

coincide for all k–schemes S and all objects g, g_1, g_2 in $\mathcal{G}(S)$ and x in $\mathcal{X}_1(S)$.

Example 5.1.6. Let a cartesian square of reductive groups over k

$$\begin{array}{ccc} G_1 & \xrightarrow{\alpha} & G_2 \\ {\scriptstyle\varphi_1}\downarrow & & \downarrow{\scriptstyle\varphi_2} \\ H_1 & \xrightarrow{\beta} & H_2 \end{array}$$

be given. Suppose that φ_1 and φ_2 are central isogenies, and denote their common kernel by μ. For each $d_1 \in \pi_1(G_1)$, the diagram

$$\begin{array}{ccc} \mathcal{M}_{G_1}^{d_1} & \xrightarrow{\alpha_*} & \mathcal{M}_{G_2}^{d_2} \\ {\scriptstyle(\varphi_1)_*}\downarrow & & \downarrow{\scriptstyle(\varphi_2)_*} \\ \mathcal{M}_{H_1}^{e_1} & \xrightarrow{\beta_*} & \mathcal{M}_{H_2}^{e_2} \end{array} \qquad \begin{array}{c} d_2 := \alpha_*(d_1) \in \pi_1(G_2) \\ \\ \\ e_\nu := (\varphi_\nu)_*(d_\nu) \in \pi_1(H_\nu) \end{array}$$

is then a morphism of torsors under the group stack $\mathcal{M}_\mu$.

Proposition 5.1.7. *Let a $\mathcal{G}$–torsor $\Phi_\nu : \mathcal{X}_\nu \longrightarrow \mathcal{Y}_\nu$ with $\Gamma(\mathcal{X}_\nu, \mathcal{O}_{\mathcal{X}_\nu}) = k$ be given for $\nu = 1, 2$, together with a morphism of $\mathcal{G}$–torsors*

$$\begin{array}{ccc} \mathcal{X}_1 & \xrightarrow{A} & \mathcal{X}_2 \\ {\scriptstyle\Phi_1}\downarrow & & \downarrow{\scriptstyle\Phi_2} \\ \mathcal{Y}_1 & \xrightarrow{B} & \mathcal{Y}_2 \end{array}$$

such that the induced morphism of Picard functors $A^* : \underline{\mathrm{Pic}}(\mathcal{X}_2) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{X}_1)$ is injective. Then the diagram of Picard functors

$$\begin{array}{ccc} \underline{\mathrm{Pic}}(\mathcal{X}_1) & \xleftarrow{A^*} & \underline{\mathrm{Pic}}(\mathcal{X}_2) \\ {\scriptstyle\Phi_1^*}\uparrow & & \uparrow{\scriptstyle\Phi_2^*} \\ \underline{\mathrm{Pic}}(\mathcal{Y}_1) & \xleftarrow{B^*} & \underline{\mathrm{Pic}}(\mathcal{Y}_2) \end{array}$$

is a pullback square.

Proof. The proof of [22, Theorem 5.7] generalises to this situation as follows. Let S be a scheme of finite type over k. For a line bundle $\mathcal{L}$ on $S \times \mathcal{X}_\nu$, we denote by $\mathrm{Lin}^{\mathcal{G}}(\mathcal{L})$ the set of its $\mathcal{G}$–linearisations, cf. [22, Definition 2.8]. According to Lemma 2.1.2(i), each automorphism of $\mathcal{L}$ comes from $\Gamma(S, \mathcal{O}_S^*)$ and hence respects each linearisation of $\mathcal{L}$. Thus [22, Theorem 4.1] provides a canonical bijection between the set $\mathrm{Lin}^{\mathcal{G}}(\mathcal{L})$ and the fibre of

$$\Phi_\nu^* : \mathrm{Pic}(S \times \mathcal{Y}_\nu) \longrightarrow \mathrm{Pic}(S \times \mathcal{X}_\nu)$$

over the isomorphism class of $\mathcal{L}$.

Let $\mathcal{T}$ be an algebraic stack over k. We denote for the moment by $\mathcal{P}ic(\mathcal{T})$ the groupoid of line bundles on $\mathcal{T}$ and their isomorphisms. Lemma 2.1.2(i) and Corollary 2.1.3 show that the functor

$$A^* : \mathcal{P}ic(\mathcal{T} \times \mathcal{X}_2) \longrightarrow \mathcal{P}ic(\mathcal{T} \times \mathcal{X}_1)$$

is fully faithful for every $\mathcal{T}$. We recall that an element in $\mathrm{Lin}^{\mathcal{G}}(\mathcal{L})$ is an isomorphism in $\mathcal{P}ic(\mathcal{G} \times S \times \mathcal{X}_\nu)$ between two pullbacks of $\mathcal{L}$ such that certain induced diagrams in $\mathcal{P}ic(S \times \mathcal{X}_\nu)$ and in $\mathcal{P}ic(\mathcal{G} \times \mathcal{G} \times S \times \mathcal{X}_\nu)$ commute. Thus it follows for all $\mathcal{L} \in \mathrm{Pic}(S \times \mathcal{X}_2)$ that the canonical map

$$A^* : \mathrm{Lin}^{\mathcal{G}}(\mathcal{L}) \longrightarrow \mathrm{Lin}^{\mathcal{G}}(A^*\mathcal{L})$$

is bijective. Hence the diagram of abelian groups

$$\begin{array}{ccc} \mathrm{Pic}(S \times \mathcal{X}_1) & \xleftarrow{A^*} & \mathrm{Pic}(S \times \mathcal{X}_2) \\ \Phi_1^* \uparrow & & \uparrow \Phi_2^* \\ \mathrm{Pic}(S \times \mathcal{Y}_1) & \xleftarrow{B^*} & \mathrm{Pic}(S \times \mathcal{Y}_2) \end{array}$$

is a pullback square, as required. □

5.2. Néron–Severi groups $\mathrm{NS}(\mathcal{M}_G^d)$ for reductive G.

Definition 5.2.1. The *Néron–Severi group* $\mathrm{NS}(\mathcal{M}_G^d)$ is the subgroup

$$\mathrm{NS}(\mathcal{M}_G^d) \subseteq \mathrm{NS}(\mathcal{M}_{Z^0}) \oplus \mathrm{NS}(\mathcal{M}_{\tilde{G}})$$

of all triples $l_Z : \Lambda_{Z^0} \longrightarrow \mathbb{Z}$, $b_Z : \Lambda_{Z^0} \otimes \Lambda_{Z^0} \longrightarrow \mathrm{End}\, J_C$ and $b : \Lambda_{T_{\tilde{G}}} \otimes \Lambda_{T_{\tilde{G}}} \longrightarrow \mathbb{Z}$ with the following properties:

(1) For every lift $\bar{\delta} \in \Lambda_{T_{\bar{G}}}$ of $\bar{d} \in \pi_1(\bar{G})$, the direct sum

$$l_Z \oplus b(-\bar{\delta} \otimes \_) : \Lambda_{Z^0} \oplus \Lambda_{T_{\tilde{G}}} \longrightarrow \mathbb{Z}$$

is integral on Λ_{T_G}.

(2) The orthogonal direct sum

$$b_Z \perp (\mathrm{id}_{J_C} \cdot b) : (\Lambda_{Z^0} \oplus \Lambda_{T_{\tilde{G}}}) \otimes (\Lambda_{Z^0} \oplus \Lambda_{T_{\tilde{G}}}) \longrightarrow \mathrm{End}\, J_C$$

is integral on $\Lambda_{T_G} \otimes \Lambda_{T_G}$.

Lemma 5.2.2. *If condition 1 above holds for one lift $\bar{\delta} \in \Lambda_{T_{\bar{G}}}$ of $\bar{d} \in \pi_1(\bar{G})$, then it holds for every lift $\bar{\delta} \in \Lambda_{T_{\bar{G}}}$ of the same element $\bar{d} \in \pi_1(\bar{G})$.*

Proof. Any two lifts $\bar{\delta}$ of $\bar{d}$ differ by some element $\lambda \in \Lambda_{T_{\tilde{G}}}$. Lemma 4.3.4 states in particular that

$$b(-\lambda \otimes \_) : \Lambda_{T_{\tilde{G}}} \longrightarrow \mathbb{Z}$$

is integral on $\Lambda_{T_{\tilde{G}}}$, and hence admits an extension $\Lambda_{T_G} \longrightarrow \mathbb{Z}$ that vanishes on Λ_{Z^0}. □

Remark 5.2.3. If G is simply connected, then $\mathrm{NS}(\mathcal{M}_G^0)$ coincides with the group $\mathrm{NS}(\mathcal{M}_G)$ of definition 4.3.2. If $G = T$ is a torus, then $\mathrm{NS}(\mathcal{M}_T^d)$ coincides for all $d \in \pi_1(T)$ with the group $\mathrm{NS}(\mathcal{M}_T)$ of definition 3.2.1.

Remark 5.2.4. The Weyl group W of (G, T_G) acts trivially on $\mathrm{NS}(\mathcal{M}_G^d)$. Hence the group $\mathrm{NS}(\mathcal{M}_G^d)$ does not depend on the choice of T_G; cf. Subsection 4.3.

Definition 5.2.5. Given a lift $\delta \in \Lambda_{T_G}$ of $d \in \pi_1(G)$, the homomorphism

$$(\iota_G)^{\mathrm{NS},\delta} : \mathrm{NS}(\mathcal{M}_G^d) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_G})$$

sends $(l_Z, b_Z) \in \mathrm{NS}(\mathcal{M}_{Z^0})$ and $b \in \mathrm{NS}(\mathcal{M}_{\widetilde{G}})$ to the pair

$$l_Z \oplus b(-\bar{\delta} \otimes \_) : \Lambda_G \longrightarrow \mathbb{Z} \quad \text{and} \quad b_Z \perp (\mathrm{id}_{J_C} \cdot b) : \Lambda_{T_G} \otimes \Lambda_{T_G} \longrightarrow \mathrm{End}\, J_C$$

where $\bar{\delta} \in \Lambda_{T_{\widetilde{G}}}$ denotes the image of δ.

Note that this definition agrees with the earlier definition 4.3.5 in the cases covered by both, namely G simply connected and $\delta \in \Lambda_{T_G}$.

Lemma 5.2.6. *Given a lift $\delta \in \Lambda_{T_G}$ of $d \in \pi_1(G)$, the diagram*

$$\begin{array}{ccccc}
\mathrm{NS}(\mathcal{M}_G^d) & & \xrightarrow{(\iota_G)^{\mathrm{NS},\delta}} & & \mathrm{NS}(\mathcal{M}_{T_G}) \\
\big\downarrow & & & & \big\downarrow {\scriptstyle (\zeta\cdot\pi)^*} \\
\mathrm{NS}(\mathcal{M}_{Z^0}) \oplus \mathrm{NS}(\mathcal{M}_{\widetilde{G}}) & \xrightarrow{\mathrm{id} \oplus (\iota_{\widetilde{G}})^{\mathrm{NS},\bar{\delta}}} & \mathrm{NS}(\mathcal{M}_{Z^0}) \oplus \mathrm{NS}(\mathcal{M}_{T_{\widetilde{G}}}) & \hookrightarrow & \mathrm{NS}(\mathcal{M}_{Z^0 \times T_{\widetilde{G}}})
\end{array}$$

is a pullback square; here $\bar{\delta} \in \Lambda_{T_{G^{ad}}}$ again denotes the image of δ.

Proof. This follows directly from the definitions. □

Let $e \in \pi_1(H)$ be the image of $d \in \pi_1(G)$ under a homomorphism of reductive groups $\varphi : G \longrightarrow H$. φ induces a map $\varphi : \widetilde{G} \longrightarrow \widetilde{H}$ between the universal covers of their commutator subgroups. If φ maps the identity component Z_G^0 in the center Z_G of G to the center Z_H of H, then it induces an obvious pullback map

$$\varphi^* : \mathrm{NS}(\mathcal{M}_H^e) \longrightarrow \mathrm{NS}(\mathcal{M}_G^d)$$

which sends l_Z, b_Z and b simply to $\varphi^* l_Z$, $\varphi^* b_Z$ and $\varphi^* b$. This is a special case of the following map, which φ induces even without the hypothesis on the centers, and which also generalises the previous definition 5.2.5.

Definition 5.2.7. Choose a maximal torus $\iota_H : T_H \hookrightarrow H$ containing $\varphi(T_G)$, and a lift $\delta \in \Lambda_{T_G}$ of $d \in \pi_1(G)$; let $\eta \in \Lambda_{T_H}$ be the image of δ. Then the map

$$\varphi^{\mathrm{NS},d} : \mathrm{NS}(\mathcal{M}_H^e) \longrightarrow \mathrm{NS}(\mathcal{M}_G^d)$$

sends $(l_Z, b_Z) \in \mathrm{NS}(\mathcal{M}_{Z_H^0})$ and $b \in \mathrm{NS}(\mathcal{M}_{\widetilde{H}})$ to the pullback along $\varphi : Z_G^0 \longrightarrow T_H$ of $(\iota_H)^{\mathrm{NS},\eta}(l_Z, b_Z, b) \in \mathrm{NS}(\mathcal{M}_{T_H})$, together with $\varphi^* b \in \mathrm{NS}(\mathcal{M}_{\widetilde{G}})$.

Lemma 5.2.8. *The map $\varphi^{\mathrm{NS},d}$ does not depend on the choice of T_G, T_H or δ.*

Proof. Let W_G denote the Weyl group of (G, T_G). It acts trivially on $\Lambda_{Z_G^0}$, and without nontrivial coinvariants on $\Lambda_{T_{\widetilde{G}}}$; these two observations imply

$$\mathrm{Hom}(\Lambda_{T_{\widetilde{G}}} \otimes \Lambda_{Z_G^0}, \mathbb{Z})^{W_G} = 0. \tag{13}$$

Lemma 4.3.4 states that b is integral on $\Lambda_{T_{\widetilde{H}}} \otimes \Lambda_{T_{\bar{H}}}$; its composition with the canonical projection $\Lambda_{T_H} \twoheadrightarrow \Lambda_{T_{\bar{H}}}$ is a Weyl–invariant map $b_r : \Lambda_{T_{\widetilde{H}}} \otimes \Lambda_{T_H} \longrightarrow \mathbb{Z}$. As explained in Subsection 4.3, Lemma 4.3.1 implies that $\varphi^* b_r : \Lambda_{T_{\widetilde{G}}} \otimes \Lambda_{T_G} \longrightarrow \mathbb{Z}$ is still Weyl–invariant; hence it vanishes on $\Lambda_{T_{\widetilde{G}}} \otimes \Lambda_{Z_G^0}$ by (13).

Any two lifts δ of d differ by some element $\lambda \in \Lambda_{T_{\widetilde{G}}}$; then the two images of $(l_Z, b_Z, b) \in \mathrm{NS}(\mathcal{M}_H^e)$ in $\mathrm{NS}(\mathcal{M}_{T_H})$ differ, according to the proof of Lemma 5.2.2, only by $b_r(-\lambda \otimes \_) : \Lambda_{T_H} \longrightarrow \mathbb{Z}$. Thus their compositions with $\varphi : \Lambda_{Z_G^0} \longrightarrow \Lambda_{T_H}$ coincide by the previous paragraph. This shows that the two images of (l_Z, b_Z, b) have the same component in the direct summand $\mathrm{Hom}(\Lambda_{Z_G^0}, \mathbb{Z})$ of $\mathrm{NS}(\mathcal{M}_G^d)$; since the other two components do not involve δ at all, the independence on δ follows.
The independence on T_G and T_H is then a consequence of Lemma 4.3.1, since the Weyl groups W_G and W_H act trivially on $\mathrm{NS}(\mathcal{M}_G^d)$ and on $\mathrm{NS}(\mathcal{M}_H^e)$. □

Lemma 5.2.9. *For all maximal tori $\iota_G : T_G \hookrightarrow G$ and $\iota_H : T_H \hookrightarrow H$ with $\varphi(T_G) \subseteq T_H$, and all lifts $\delta \in \Lambda_{T_G}$ of $d \in \pi_1(G)$, the diagram*

$$\begin{array}{ccc} \mathrm{NS}(\mathcal{M}_H^e) & \xrightarrow{(\iota_H)^{\mathrm{NS},\eta}} & \mathrm{NS}(\mathcal{M}_{T_H}) \\ \downarrow{\scriptstyle \varphi^{\mathrm{NS},d}} & & \downarrow{\scriptstyle \varphi^*} \\ \mathrm{NS}(\mathcal{M}_G^d) & \xrightarrow{(\iota_G)^{\mathrm{NS},\delta}} & \mathrm{NS}(\mathcal{M}_{T_G}) \end{array}$$

commutes, with $\eta := \varphi_*\delta \in \Lambda_{T_H}$ and $e := \varphi_* d \in \pi_1(H)$ as in definition 5.2.7.

Proof. Given an element in $\mathrm{NS}(\mathcal{M}_H^e)$, we have to compare its two images in $\mathrm{NS}(\mathcal{M}_{T_G})$. The definition 5.2.7 of $\varphi^{\mathrm{NS},d}$ directly implies that both have the same pullback to $\mathrm{NS}(\mathcal{M}_{Z_G^0})$ and to $\mathrm{NS}(\mathcal{M}_{T_{\widetilde{G}}})$. Moreover, their components in the direct summand $\mathrm{Hom}^s(\Lambda_{T_G} \otimes \Lambda_{T_G}, \mathrm{End}\, J_C)$ of $\mathrm{NS}(\mathcal{M}_{T_G})$ are both Weyl–invariant due to Lemma 4.3.1; thus equation (13) above shows that these components vanish on $\Lambda_{T_{\widetilde{G}}} \otimes \Lambda_{Z_G^0}$ and on $\Lambda_{Z_G^0} \otimes \Lambda_{T_{\widetilde{G}}}$. Hence two images in question even have the same pullback to $\mathrm{NS}(\mathcal{M}_{Z_G^0 \times T_{\widetilde{G}}})$. But $\Lambda_{Z_G^0} \oplus \Lambda_{T_{\widetilde{G}}}$ has finite index in Λ_{T_G}. □

Corollary 5.2.10. *Let $\psi : H \longrightarrow K$ be another homomorphism of reductive groups, and put $f := \psi_* e \in \pi_1(K)$. Then*

$$\varphi^{\mathrm{NS},d} \circ \psi^{\mathrm{NS},e} = (\psi \circ \varphi)^{\mathrm{NS},d} : \mathrm{NS}(\mathcal{M}_K^f) \longrightarrow \mathrm{NS}(\mathcal{M}_G^d).$$

Proof. According to the previous lemma, this equality holds after composition with $(\iota_G)^{\mathrm{NS},\delta} : \mathrm{NS}(\mathcal{M}_G^d) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_G})$ for any lift $\delta \in \Lambda_{T_G}$ of d. Due to the Lemma 4.3.6 and Lemma 5.2.6, there is a lift δ of d such that $(\iota_G)^{\mathrm{NS},\delta}$ is injective. □

We conclude this subsection with a more explicit description of $\mathrm{NS}(\mathcal{M}_G^d)$. It turns out that genus $g_C = 0$ is special. This generalises the description obtained for $k = \mathbb{C}$ and G semisimple by different methods in [31, Section V].

Proposition 5.2.11. *Let $q : G \twoheadrightarrow G/G' =: G^{ab}$ denote the maximal abelian quotient of G. Then the sequence of abelian groups*

$$0 \longrightarrow \mathrm{NS}(\mathcal{M}_{G^{ab}}) \xrightarrow{q^*} \mathrm{NS}(\mathcal{M}_G^d) \xrightarrow{\mathrm{pr}_2} \mathrm{NS}(\mathcal{M}_{\widetilde{G}})$$

is exact, and the image of the map pr_2 *in it consists of all forms* $b : \Lambda_{T_{\tilde{G}}} \otimes \Lambda_{T_{\tilde{G}}} \longrightarrow \mathbb{Z}$ *in* $\mathrm{NS}(\mathcal{M}_{\tilde{G}})$ *that are integral*

- *on* $\Lambda_{T_{\tilde{G}}} \otimes \Lambda_{T_{G'}}$*, if* $g_C \geq 1$*;*
- *on* $(\mathbb{Z}\bar{\delta}) \otimes \Lambda_{T_{G'}}$ *for a lift* $\bar{\delta} \in \Lambda_{T_{\tilde{G}}}$ *of* $\bar{d} \in \pi_1(\bar{G})$*, if* $g_C = 0$*.*

The condition does not depend on the choice of this lift $\bar{\delta}$*, due to Lemma 4.3.4.*

Proof. Since $q : Z^0 \longrightarrow G^{\mathrm{ab}}$ is an isogeny, q^* is injective; it clearly maps into the kernel of pr_2. Conversely, let $(l_Z, b_Z, b) \in \mathrm{NS}(\mathcal{M}_G^d)$ be in the kernel of pr_2; this means $b = 0$. Then condition 1 in the definition 5.2.1 of $\mathrm{NS}(\mathcal{M}_G^d)$ provides a map

$$l_Z \oplus 0 : \Lambda_{T_G} \longrightarrow \mathbb{Z}$$

which vanishes on $\Lambda_{T_{\tilde{G}}}$, and hence also on $\Lambda_{T_{G'}}$; thus it is induced from a map on $\Lambda_{T_G}/\Lambda_{T_{G'}} = \Lambda_{G^{\mathrm{ab}}}$. Similarly, condition 2 in the same definition provides a map $b_Z \perp 0$ on $\Lambda_{T_G} \otimes \Lambda_{T_G}$ which vanishes on $\Lambda_{T_{\tilde{G}}} \otimes \Lambda_{T_G} + \Lambda_{T_G} \otimes \Lambda_{T_{\tilde{G}}}$, and hence also on $\Lambda_{T_{G'}} \otimes \Lambda_{T_G} + \Lambda_{T_G} \otimes \Lambda_{T_{G'}}$; thus it is induced from a map on the quotient $\Lambda_{G^{\mathrm{ab}}} \otimes \Lambda_{G^{\mathrm{ab}}}$. This proves the exactness.
Now let $b \in \mathrm{NS}(\mathcal{M}_{\tilde{G}}^d)$ be in the image of pr_2. Then b is integral on $(\mathbb{Z}\bar{\delta}) \otimes \Lambda_{G'}$ by condition 1 in definition 5.2.1. If $g_C \geq 1$, then

$$\_ \cdot \mathrm{id}_{J_C} : \mathbb{Z} \longrightarrow \mathrm{End}\, J_C$$

is injective with torsionfree cokernel; thus condition 2 in definition 5.2.1 implies that

$$0 \oplus b : (\Lambda_{Z^0} \oplus \Lambda_{T_{\tilde{G}}}) \otimes \Lambda_{T_{\tilde{G}}} \longrightarrow \mathbb{Z}$$

is integral on $\Lambda_{T_G} \otimes \Lambda_{T_{G'}}$ and hence, vanishing on $\Lambda_{Z^0} \subseteq \Lambda_{T_G}$, comes from a map on the quotient $\Lambda_{T_{\tilde{G}}} \otimes \Lambda_{T_{G'}}$. This shows that b satisfies the stated condition.
Conversely, suppose that $b \in \mathrm{NS}(\mathcal{M}_{\tilde{G}}^d)$ satisfies the stated condition. Then b is integral on $(\mathbb{Z}\bar{\delta}) \otimes \Lambda_{T_{G'}}$; since $\Lambda_{T_{G'}} \subseteq \Lambda_{T_G}$ is a direct summand,

$$b(-\bar{\delta} \otimes \_) : \Lambda_{T_{G'}} \longrightarrow \mathbb{Z}$$

can thus be extended to Λ_{T_G}. We restrict it to a map $l_Z : \Lambda_{Z^0} \longrightarrow \mathbb{Z}$. In the case $g_C = 0$, the triple $(l_Z, 0, b)$ is in $\mathrm{NS}(\mathcal{M}_G^d)$ and hence an inverse image of b. It remains to consider $g_C \geq 1$. Then b is by assumption integral on $\Lambda_{T_{\tilde{G}}} \otimes \Lambda_{T_{G'}}$, so composing it with the canonical subjection $\Lambda_{T_G} \twoheadrightarrow \Lambda_{T_{\tilde{G}}}$ defines a linear map $\Lambda_{T_G} \otimes \Lambda_{T_{G'}} \longrightarrow \mathbb{Z}$. Since b is symmetric, this extends canonically to a symmetric linear map from

$$\Lambda_{T_G} \otimes \Lambda_{T_{G'}} + \Lambda_{T_{G'}} \otimes \Lambda_{T_G} \subseteq \Lambda_{T_G} \otimes \Lambda_{T_G}$$

to $\mathbb{Z}$. It can be extended further to a symmetric linear map from $\Lambda_{T_G} \otimes \Lambda_{T_G}$ to $\mathbb{Z}$, because $\Lambda_{T_{G'}} \subseteq \Lambda_{T_G}$ is a direct summand. Multiplying it with id_{J_C} and restricting to Λ_{Z^0} defines an element $b_Z \in \mathrm{Hom}^s(\Lambda_{Z^0} \otimes \Lambda_{Z^0}, \mathrm{End}\, J_C)$. By construction, the triple (l_Z, b_Z, b) is in $\mathrm{NS}(\mathcal{M}_G^d)$ and hence an inverse image of b. □

In particular, the free abelian group $\mathrm{NS}(\mathcal{M}_G^d)$ has rank

$$\operatorname{rk}\mathrm{NS}(\mathcal{M}_G^d) = r + r\cdot \operatorname{rk}\mathrm{NS}(J_C) + \frac{r(r-1)}{2}\cdot \operatorname{rk}\mathrm{End}(J_C) + s$$

if $G^{\mathrm{ab}} \cong \mathbb{G}_m^r$ is a torus of rank r, and G^{ad} contains s simple factors.

5.3. Proof of the main result.

Theorem 5.3.1. i) *$\Gamma(\mathcal{M}_G^d, \mathcal{O}_{\mathcal{M}_G^d}) = k$.*

ii) *The functor $\underline{\mathrm{Pic}}(\mathcal{M}_G^d)$ is representable by a k–scheme locally of finite type.*

iii) *There is a canonical exact sequence*

$$0 \longrightarrow \underline{\mathrm{Hom}}(\pi_1(G), J_C) \xrightarrow{j_G} \underline{\mathrm{Pic}}(\mathcal{M}_G^d) \xrightarrow{c_G} \mathrm{NS}(\mathcal{M}_G^d) \longrightarrow 0$$

of commutative group schemes over k.

iv) *For every homomorphism of reductive groups $\varphi : G \longrightarrow H$, the diagram*

$$\begin{array}{ccccccccc} 0 & \longrightarrow & \underline{\mathrm{Hom}}(\pi_1(H), J_C) & \xrightarrow{j_H} & \underline{\mathrm{Pic}}(\mathcal{M}_H^e) & \xrightarrow{c_H} & \mathrm{NS}(\mathcal{M}_H^e) & \longrightarrow & 0 \\ & & \downarrow{\scriptstyle \varphi^*} & & \downarrow{\scriptstyle \varphi^*} & & \downarrow{\scriptstyle \varphi^{\mathrm{NS},d}} & & \\ 0 & \longrightarrow & \underline{\mathrm{Hom}}(\pi_1(G), J_C) & \xrightarrow{j_G} & \underline{\mathrm{Pic}}(\mathcal{M}_G^d) & \xrightarrow{c_G} & \mathrm{NS}(\mathcal{M}_G^d) & \longrightarrow & 0 \end{array}$$

commutes; here $e := \varphi_*(d) \in \pi_1(H)$.

Proof. We record for later use the commutative square of abelian groups

$$\begin{array}{ccc} \pi_1(G) & \xleftarrow{\mathrm{pr}} & \Lambda_{T_G} \\ \uparrow{\scriptstyle \zeta_*} & & \uparrow{\scriptstyle (\zeta\cdot\pi)_*} \\ \Lambda_{Z^0} & \xleftarrow{\mathrm{pr}_1} & \Lambda_{Z^0 \times T_{\widetilde{G}}}. \end{array}$$

The mapping cone of this commutative square

$$(14) \qquad 0 \longrightarrow \Lambda_{Z^0} \oplus \Lambda_{T_{\widetilde{G}}} \longrightarrow \Lambda_{Z^0} \oplus \Lambda_{T_G} \longrightarrow \pi_1(G) \longrightarrow 0$$

is exact, because its subsequence $0 \longrightarrow \Lambda_{T_{\widetilde{G}}} \longrightarrow \Lambda_{T_G} \longrightarrow \pi_1(G) \longrightarrow 0$ is exact, and the resulting sequence of quotients $0 \longrightarrow \Lambda_{Z^0} = \Lambda_{Z^0} \longrightarrow 0 \longrightarrow 0$ is also exact.

Lemma 5.3.2. *There is an exact sequence of reductive groups*

$$(15) \qquad 1 \longrightarrow \widetilde{G} \longrightarrow \widehat{G} \xrightarrow{\mathrm{dt}} \mathbb{G}_m \longrightarrow 1$$

and an extension $\widehat{\pi} : \widehat{G} \longrightarrow G$ of $\pi : \widetilde{G} \longrightarrow G$ such that $\widehat{\pi}_* : \pi_1(\widehat{G}) \longrightarrow \pi_1(G)$ maps $1 \in \mathbb{Z} = \pi_1(\mathbb{G}_m) = \pi_1(\widehat{G})$ to the given element $d \in \pi_1(G)$.

Proof. We view the given $d \in \pi_1(G)$ as a coset $d \subseteq \Lambda_{T_G}$ modulo $\Lambda_{\mathrm{coroots}}$. Let

$$\Lambda_{T_{\widehat{G}}} \subseteq \Lambda_{T_G} \oplus \mathbb{Z}$$

be generated by $\Lambda_{\mathrm{coroots}} \oplus 0$ and $(d, 1)$, and let

$$(\widehat{\pi}, \mathrm{dt}) : \widehat{G} \longrightarrow G \times \mathbb{G}_m$$

be the reductive group with the same root system as G, whose maximal torus $T_{\widehat{G}} = \widehat{\pi}^{-1}(T_G)$ has cocharacter lattice $\mathrm{Hom}(\mathbb{G}_m, T_{\widehat{G}}) = \Lambda_{T_{\widehat{G}}}$. As π_* maps $\Lambda_{T_{\widetilde{G}}}$ isomorphically onto $\Lambda_{\mathrm{coroots}}$, we obtain an exact sequence

$$0 \longrightarrow \Lambda_{T_{\widetilde{G}}} \xrightarrow{\pi_*} \Lambda_{T_{\widehat{G}}} \xrightarrow{\mathrm{pr}_2} \mathbb{Z} \longrightarrow 0,$$

which yields the required exact sequence (15) of groups. By its construction, $\widehat{\pi}_*$ maps the canonical generator $1 \in \pi_1(\mathbb{G}_m) = \pi_1(\widehat{G})$ to $d \in \pi_1(G)$. $\square$

Let μ denote the kernel of the central isogeny $\zeta \cdot \pi : Z^0 \times \widetilde{G} \twoheadrightarrow G$. Then

$$\psi : Z^0 \times \widehat{G} \longrightarrow G \times \mathbb{G}_m, \qquad (z^0, \widehat{g}) \longmapsto \big(\zeta(z^0) \cdot \widehat{\pi}(\widehat{g}), \mathrm{dt}(\widehat{g})\big)$$

is by construction a central isogeny with kernel μ. Hence the induced 1–morphism

$$\psi_* : \mathcal{M}^0_{Z^0} \times \mathcal{M}^1_{\widehat{G}} \longrightarrow \mathcal{M}^d_G \times \mathcal{M}^1_{\mathbb{G}_m}$$

is faithfully flat by Lemma 2.2.2. Restricting to the point $\mathrm{Spec}(k) \longrightarrow \mathcal{M}^1_{\mathbb{G}_m}$ given by a line bundle L of degree 1 on C, we get a faithfully flat 1–morphism

$$(\psi_*)_L : \mathcal{M}^0_{Z^0} \times \mathcal{M}_{\widehat{G},L} \longrightarrow \mathcal{M}^d_G.$$

Since $\Gamma(\mathcal{M}^0_{Z^0} \times \mathcal{M}_{\widehat{G},L}, \mathcal{O}) = k$ by Proposition 4.4.7(i) and Lemma 2.1.2(i), part (i) of the theorem follows. The group stack $\mathcal{M}_\mu$ acts by tensor product on these two 1–morphisms ψ_* and $(\psi_*)_L$, turning both into $\mathcal{M}_\mu$–torsors; cf. Example 5.1.4. The idea is to descend line bundles along the torsor $(\psi_*)_L$.

We choose a principal $T_{\widehat{G}}$–bundle $\widehat{\xi}$ on C together with an isomorphism of line bundles $\mathrm{dt}_* \widehat{\xi} \cong L$. Then $\xi := \widehat{\pi}_*(\widehat{\xi})$ is a principal T_G–bundle on C; their degrees $\widehat{\delta} := \deg(\widehat{\xi}) \in \Lambda_{T_{\widehat{G}}}$ and $\delta := \deg(\xi) \in \Lambda_{T_G}$ are lifts of $d \in \pi_1(G)$. The diagram

$$\begin{array}{ccc} Z^0 \times T_{\widehat{G}} & \xrightarrow{\mathrm{id} \times \iota_{\widehat{G}}} & Z^0 \times \widehat{G} \\ \downarrow{\scriptstyle \psi} & & \downarrow{\scriptstyle \psi} \\ T_G \times \mathbb{G}_m & \xrightarrow{\iota_G \times \mathrm{id}} & G \times \mathbb{G}_m \end{array} \tag{16}$$

of groups induces the right square in the 2–commutative diagram

$$\begin{array}{ccccc} \mathcal{M}^0_{Z^0} \times \mathcal{M}^0_{T_{\widehat{G}}} & \xrightarrow{\mathrm{id} \times t_{\widehat{\xi}}} & \mathcal{M}^0_{Z^0} \times \mathcal{M}^{\widehat{\delta}}_{T_{\widehat{G}}} & \xrightarrow{(\mathrm{id} \times \iota_{\widehat{G}})_*} & \mathcal{M}^0_{Z^0} \times \mathcal{M}^1_{\widehat{G}} \\ \downarrow{\scriptstyle \psi_*} & & \downarrow{\scriptstyle \psi_*} & & \downarrow{\scriptstyle \psi_*} \\ \mathcal{M}^0_{T_G} \times \mathcal{M}^1_{\mathbb{G}_m} & \xrightarrow{t_\xi \times \mathrm{id}} & \mathcal{M}^\delta_{T_G} \times \mathcal{M}^1_{\mathbb{G}_m} & \xrightarrow{(\iota_G \times \mathrm{id})_*} & \mathcal{M}^d_G \times \mathcal{M}^1_{\mathbb{G}_m} \end{array} \tag{17}$$

of moduli stacks; note that $t_{\widehat{\xi}}$ and t_{ξ} are equivalences. Restricting the outer rectangle again to the point $\mathrm{Spec}(k) \longrightarrow \mathcal{M}^1_{\mathbb{G}_m}$ given by L, we get the diagram

$$\begin{array}{ccccc} \mathcal{M}^0_{Z^0 \times T_{\widetilde{G}}} & \xrightarrow{\sim} & \mathcal{M}^0_{Z^0} \times \mathcal{M}^0_{T_{\widetilde{G}}} & \xrightarrow{\mathrm{id} \times \iota_{\widehat{\xi}}} & \mathcal{M}^0_{Z^0} \times \mathcal{M}_{\widehat{G},L} \\ & {\scriptstyle (\zeta\cdot\pi)_*} \searrow & \downarrow{\scriptstyle \zeta_* \otimes \pi_*} & & \downarrow{\scriptstyle (\psi_*)_L} \\ & & \mathcal{M}^0_{T_G} & \xrightarrow{(\iota_G)_* \circ t_{\xi}} & \mathcal{M}^d_G \end{array} \tag{18}$$

containing an instance $\iota_{\widehat{\xi}}$ of the 1–morphism (10) defined in Subsection 4.4. According to the Proposition 3.2.2 and Proposition 4.4.7,

$$\iota^*_{\widehat{\xi}} : \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{M}^0_{T_{\widetilde{G}}})$$

is a morphism of group schemes over k. This morphism is a closed immersion, according to Proposition 4.4.7(iii), if $g_C \geq 1$ or if $\widehat{\xi}$ is chosen appropriately, as explained in Lemma 4.3.6; we assume this in the sequel. Using Lemma 2.1.4 and Corollary 3.2.4, it follows that

$$(\mathrm{id} \times \iota_{\widehat{\xi}})^* : \underline{\mathrm{Pic}}(\mathcal{M}^0_{Z^0}) \oplus \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) \cong \underline{\mathrm{Pic}}(\mathcal{M}^0_{Z^0} \times \mathcal{M}_{\widehat{G},L}) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{M}^0_{Z^0 \times T_{\widetilde{G}}})$$

is a closed immersion of group schemes over k as well.
The group stack $\mathcal{M}_{\mu}$ still acts by tensor product on the vertical 1–morphisms in (17) and in (18). Since the diagram (16) of groups is cartesian, (17) and (18) are morphisms of $\mathcal{G}$–torsors; cf. Example 5.1.6. Proposition 5.1.7 applies to the latter morphism of torsors, yielding a cartesian square

$$\begin{array}{ccc} \underline{\mathrm{Pic}}(\mathcal{M}^d_G) & \xrightarrow{t^*_{\xi} \circ \iota^*_G} & \underline{\mathrm{Pic}}(\mathcal{M}^0_{T_G}) \\ \downarrow{\scriptstyle \psi^*_L} & & \downarrow{\scriptstyle (\zeta\cdot\pi)^*} \\ \underline{\mathrm{Pic}}(\mathcal{M}^0_{Z^0}) \oplus \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L}) & \xrightarrow{(\mathrm{id} \times \iota_{\widehat{\xi}})^*} & \underline{\mathrm{Pic}}(\mathcal{M}^0_{Z^0 \times T_{\widetilde{G}}}) \end{array} \tag{19}$$

of Picard functors. Thus $\underline{\mathrm{Pic}}(\mathcal{M}^d_G)$ is representable, and $t^*_{\xi} \circ \iota^*_G$ is a closed immersion; this proves part (ii) of the theorem.
The image of the mapping cone (14) under the exact functor $\underline{\mathrm{Hom}}(\_, J_C)$, and the mapping cones of the two cartesian squares given by diagram (19) and Lemma 5.2.6, are the columns of the commutative diagram

$$\begin{array}{ccccccccc}
 & & 0 & & 0 & & 0 & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & \underline{\mathrm{Hom}}(\pi_1(G), J_C) & & \underline{\mathrm{Pic}}(\mathcal{M}_G^d) & & \mathrm{NS}(\mathcal{M}_G^d) & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & \begin{matrix}\underline{\mathrm{Hom}}(\Lambda_{Z^0}, J_C)\\ \oplus \\ \underline{\mathrm{Hom}}(\Lambda_{T_G}, J_C)\end{matrix} & \xrightarrow{j_{Z^0} \oplus j_{T_G}} & \begin{matrix}\underline{\mathrm{Pic}}(\mathcal{M}_{Z^0}^0)\\ \oplus \\ \underline{\mathrm{Pic}}(\mathcal{M}_{\widehat{G},L})\\ \oplus \\ \underline{\mathrm{Pic}}(\mathcal{M}_{T_G}^0)\end{matrix} & \xrightarrow{c_{Z^0} \oplus c_{\widetilde{G}} \oplus c_{T_G}} & \begin{matrix}\mathrm{NS}(\mathcal{M}_{Z^0})\\ \oplus \\ \mathrm{NS}(\mathcal{M}_{\widetilde{G}})\\ \oplus \\ \mathrm{NS}(\mathcal{M}_{T_G})\end{matrix} & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & \underline{\mathrm{Hom}}(\Lambda_{Z^0 \times T_{\widetilde{G}}}, J_C) & \xrightarrow{j_{Z^0 \times T_{\widetilde{G}}}} & \underline{\mathrm{Pic}}(\mathcal{M}_{Z^0 \times T_{\widetilde{G}}}^0) & \xrightarrow{c_{Z^0 \times T_{\widetilde{G}}}} & \mathrm{NS}(\mathcal{M}_{Z^0 \times T_{\widetilde{G}}}) & \longrightarrow & 0 \\
 & & \downarrow & & & & & & \\
 & & 0 & & & & & &
\end{array}$$

whose two rows are exact due to Proposition 3.2.2(ii) and Proposition 4.4.7(ii). Applying the snake lemma to this diagram, we get an exact sequence

$$0 \longrightarrow \underline{\mathrm{Hom}}(\pi_1(G), J_C) \xrightarrow{j_G(\iota_G, \delta)} \underline{\mathrm{Pic}}(\mathcal{M}_G^d) \xrightarrow{c_G(\iota_G, \delta)} \mathrm{NS}(\mathcal{M}_G^d) \longrightarrow 0.$$

The image of $j_G(\iota_G, \delta)$ and the kernel of $c_G(\iota_G, \delta)$ are a priori independent of the choices made, since both are the largest quasicompact open subgroup in $\underline{\mathrm{Pic}}(\mathcal{M}_G^d)$. If G is a torus and $d = 0$, then this is the exact sequence of Proposition 3.2.2; in general, the construction provides a morphism of exact sequences

(20)

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \underline{\mathrm{Hom}}(\pi_1(G), J_C) & \xrightarrow{j_G(\iota_G, \delta)} & \underline{\mathrm{Pic}}(\mathcal{M}_G^d) & \xrightarrow{c_G(\iota_G, \delta)} & \mathrm{NS}(\mathcal{M}_G^d) & \longrightarrow & 0 \\
 & & \downarrow{\scriptstyle \mathrm{pr}^*} & & \downarrow{\scriptstyle t_\xi^* \circ \iota_G^*} & & \downarrow{\scriptstyle (\iota_G)^{\mathrm{NS}, \delta}} & & \\
0 & \longrightarrow & \underline{\mathrm{Hom}}(\Lambda_{T_G}, J_C) & \xrightarrow{j_{T_G}} & \underline{\mathrm{Pic}}(\mathcal{M}_{T_G}^0) & \xrightarrow{c_{T_G}} & \mathrm{NS}(\mathcal{M}_{T_G}) & \longrightarrow & 0
\end{array}$$

whose three vertical maps are all injective. Using Proposition 3.2.2(iii), this implies that $j_G(\iota_G, \delta)$ and $c_G(\iota_G, \delta)$ depend at most on the choice of $\iota_G : T_G \hookrightarrow G$ and of δ, but not on the choice of $\widehat{G}$, L or $\widehat{\xi}$; thus the notation. Together with the following two lemmas, this proves the remaining parts (iii) and (iv) of the theorem. □

Lemma 5.3.3. *The above map* $j_G(\iota_G, \delta) : \underline{\mathrm{Hom}}(\pi_1(G), J_C) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{M}_G^d)$

i) *does not depend on the lift* $\delta \in \Lambda_{T_G}$ *of* $d \in \pi_1(G)$,
ii) *does not depend on the maximal torus* $\iota_G : T_G \hookrightarrow G$, *and*
iii) *satisfies* $\varphi^* \circ j_H = j_G \circ \varphi^* : \underline{\mathrm{Hom}}(\pi_1(H), J_C) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{M}_G^d)$ *for all* $\varphi : G \longrightarrow H$.

Proof. If G is a torus, then δ and ι_G are unique, so (i) and (ii) hold trivially. The claim is empty for $g_C = 0$, so we assume $g_C \geq 1$. Then the above construction works for all lifts δ of d, because $\iota^*_{\widehat{\xi}}$ is a closed immersion for all $\widehat{\xi}$.

Given $\varphi : G \longrightarrow H$ and a maximal torus $\iota_H : T_H \hookrightarrow H$ with $\varphi(T_G) \subseteq T_H$, we again put $e := \varphi_* d \in \pi_1(H)$ and $\eta := \varphi_* \delta \in \Lambda_{T_H}$. Then the diagram

$$\begin{array}{ccc} \underline{\mathrm{Hom}}(\pi_1(H), J_C) & \xrightarrow{j_H(\iota_H,\eta)} & \underline{\mathrm{Pic}}(\mathcal{M}^e_H) \\ \downarrow \varphi^* & & \downarrow \varphi^* \\ \underline{\mathrm{Hom}}(\pi_1(G), J_C) & \xrightarrow{j_G(\iota_G,\delta)} & \underline{\mathrm{Pic}}(\mathcal{M}^d_G) \end{array} \tag{21}$$

commutes, because it commutes after composition with the closed immersion

$$t^*_\xi \circ \iota^*_G : \underline{\mathrm{Pic}}(\mathcal{M}^d_G) \longrightarrow \underline{\mathrm{Pic}}(\mathcal{M}^0_{T_G})$$

from diagram (20), using Remark 3.2.3. In particular, (iii) follows from (i) and (ii).

i) For $G = \mathrm{GL}_2$, it suffices to take $\varphi = \det : \mathrm{GL}_2 \longrightarrow \mathbb{G}_m$ in the above diagram (21), since $\det_* : \pi_1(\mathrm{GL}_2) \longrightarrow \pi_1(\mathbb{G}_m)$ is an isomorphism.

For $G = \mathrm{PGL}_2$, it then suffices to take $\varphi = \mathrm{pr} : \mathrm{GL}_2 \twoheadrightarrow \mathrm{PGL}_2$ in the same diagram (21), since $\mathrm{pr}_* : \pi_1(\mathrm{GL}_2) \longrightarrow \pi_1(\mathrm{PGL}_2)$ is surjective.

As (i) holds trivially for $G = \mathrm{SL}_2$, and clearly holds for $G \times \mathbb{G}_m$ if it holds for G, this proves (i) for all groups G of semisimple rank one.

In the general case, let $\alpha^\vee \in \Lambda_{T_G}$ be a coroot, and let $\varphi : G_\alpha \hookrightarrow G$ be the corresponding subgroup of semisimple rank one. Then the diagram (21) shows $j_G(\iota_G, \delta) = j_G(\iota_G, \delta + \alpha^\vee)$, since $\varphi_* : \pi_1(G_\alpha) \longrightarrow \pi_1(G)$ is surjective. This completes the proof of i, because any two lifts δ of d differ by a sum of coroots.

ii) now follows from Weyl–invariance; cf. Subsection 4.3. □

Lemma 5.3.4. *The above map* $c_G(\iota_G, \delta) : \underline{\mathrm{Pic}}(\mathcal{M}^d_G) \longrightarrow \mathrm{NS}(\mathcal{M}^d_G)$

i) *does not depend on the lift* $\delta \in \Lambda_{T_G}$ *of* $d \in \pi_1(G)$,
ii) *does not depend on the maximal torus* $\iota_G : T_G \hookrightarrow G$, *and*
iii) *satisfies* $\varphi^{\mathrm{NS},d} \circ c_H = c_G \circ \varphi^* : \underline{\mathrm{Pic}}(\mathcal{M}^e_H) \longrightarrow \mathrm{NS}(\mathcal{M}^d_G)$ *for all* $\varphi : G \longrightarrow H$.

Proof. If G is a torus, then δ and ι_G are unique; if G is simply connected, then $c_G(\iota_G, \delta)$ coincides by construction with the isomorphism c_G of Proposition 4.4.7(ii). In both cases, (i) and (ii) follow, and we can use the notation c_G without ambiguity.

Given a representation $\rho : G \longrightarrow \mathrm{SL}(V)$, the diagram

$$\begin{array}{ccc} \underline{\mathrm{Pic}}(\mathcal{M}_{\mathrm{SL}(V)}) & \xrightarrow{c_{\mathrm{SL}(V)}} & \mathrm{NS}(\mathcal{M}_{\mathrm{SL}(V)}) \\ \downarrow \rho^* & & \downarrow \rho^{\mathrm{NS},d} \\ \underline{\mathrm{Pic}}(\mathcal{M}^d_G) & \xrightarrow{c_G(\iota_G,\delta)} & \mathrm{NS}(\mathcal{M}^d_G) \end{array} \tag{22}$$

commutes, because it commutes after composition with the injective map

$$(\iota_G)^{\mathrm{NS},\delta} : \mathrm{NS}(\mathcal{M}^d_G) \longrightarrow \mathrm{NS}(\mathcal{M}_{T_G})$$

from diagram (20), using Lemma 5.2.9, Corollary 4.4.2, Remark 3.2.3, and the 2–commutative squares

$$\begin{array}{ccccc} \mathcal{M}^0_{T_G} & \xrightarrow{t_\xi} & \mathcal{M}^\delta_{T_G} & \xrightarrow{(\iota_G)_*} & \mathcal{M}^d_G \\ \downarrow{\scriptstyle \rho_*} & & \downarrow{\scriptstyle \rho_*} & & \downarrow{\scriptstyle \rho_*} \\ \mathcal{M}^0_{T_{\mathrm{SL}(V)}} & \xrightarrow{t_{\rho_*\xi}} & \mathcal{M}^{\rho_*\delta}_{T_{\mathrm{SL}(V)}} & \xrightarrow{\iota_*} & \mathcal{M}_{\mathrm{SL}(V)}) \end{array}$$

in which $\iota : T_{\mathrm{SL}(V)} \hookrightarrow \mathrm{SL}(V)$ is a maximal torus containing $\rho(T_G)$.

Similarly, given a homomorphism $\chi : G \longrightarrow T$ to a torus T, the diagram

$$\begin{array}{ccc} \underline{\mathrm{Pic}}(\mathcal{M}^{\chi_* d}_T) & \xrightarrow{c_T} & \mathrm{NS}(\mathcal{M}_T) \\ \downarrow{\scriptstyle \chi^*} & & \downarrow{\scriptstyle \chi^*} \\ \underline{\mathrm{Pic}}(\mathcal{M}^d_G) & \xrightarrow{c_G(\iota_G,\delta)} & \mathrm{NS}(\mathcal{M}^d_G) \end{array} \tag{23}$$

commutes, again because it commutes after composition with the same injective map $(\iota_G)^{\mathrm{NS},\delta}$ from diagram (20), using Lemma 5.2.9, Remark 3.2.3, and the 2–commutative squares

$$\begin{array}{ccccc} \mathcal{M}^0_{T_G} & \xrightarrow{t_\xi} & \mathcal{M}^\delta_{T_G} & \xrightarrow{(\iota_G)_*} & \mathcal{M}^d_G \\ \downarrow{\scriptstyle \chi_*} & & \downarrow{\scriptstyle \chi_*} & & \downarrow{\scriptstyle \chi_*} \\ \mathcal{M}^0_T & \xrightarrow{t_{\chi_*\xi}} & \mathcal{M}^{\chi_*\delta}_T & = & \mathcal{M}^{\chi_*\delta}_T. \end{array}$$

The two commutative diagrams (22) and (23) show that the restriction of $c_G(\iota_G, \delta)$ to the images of all ρ^* and all χ^* in $\underline{\mathrm{Pic}}(\mathcal{M}^d_G)$ modulo $\underline{\mathrm{Hom}}(\pi_1(G), J_C)$ does not depend on the choice of δ or ι_G. But these images generate a subgroup of finite index, according to Proposition 5.2.11 and Remark 4.3.3. Thus (i) and (ii) follow. The functoriality in (iii) is proved similarly; it suffices to apply these arguments to homomorphisms $\rho : H \longrightarrow \mathrm{SL}(V)$, $\chi : H \longrightarrow T$ and their compositions with $\varphi : G \longrightarrow H$, using Corollary 5.2.10. $\square$

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Singular Bott-Chern Classes and the Arithmetic Grothendieck Riemann Roch Theorem for Closed Immersions

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Abstract. We study the singular Bott-Chern classes introduced by Bismut, Gillet and Soulé. Singular Bott-Chern classes are the main ingredient to define direct images for closed immersions in arithmetic K-theory. In this paper we give an axiomatic definition of a theory of singular Bott-Chern classes, study their properties, and classify all possible theories of this kind. We identify the theory defined by Bismut, Gillet and Soulé as the only one that satisfies the additional condition of being homogeneous. We include a proof of the arithmetic Grothendieck-Riemann-Roch theorem for closed immersions that generalizes a result of Bismut, Gillet and Soulé and was already proved by Zha. This result can be combined with the arithmetic Grothendieck-Riemann-Roch theorem for submersions to extend this theorem to arbitrary projective morphisms. As a byproduct of this study we obtain two results of independent interest. First, we prove a Poincaré lemma for the complex of currents with fixed wave front set, and second we prove that certain direct images of Bott-Chern classes are closed.

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Contents

0 Introduction

Chern-Weil theory associates to each hermitian vector bundle a family of closed characteristic forms that represent the characteristic classes of the vector bundle. The characteristic classes are compatible with exact sequences. But this is not true for the characteristic forms. The Bott-Chern classes measure the lack of compatibility of the characteristic forms with exact sequences.

The Grothendieck-Riemann-Roch theorem gives a formula that relates direct images and characteristic classes. In general this formula is not valid for the characteristic forms. The singular Bott-Chern classes measure, in a functorial way, the failure of an exact Grothendieck-Riemann-Roch theorem for closed immersions at the level of characteristic forms. In the same spirit, the analytic torsion forms measure the failure of an exact Grothendieck-Riemann-Roch theorem for submersions at the level of characteristic forms. Hence singular Bott-Chern classes and analytic torsion forms are analogous objects, the first for closed immersions and the second for submersions.

Let us give a more precise description of Bott-Chern classes and singular Bott-Chern classes. Let X be a complex manifold and let φ be a symmetric power series in r variables with real coefficients. Let $\overline{E} = (E, h)$ be a rank r holomorphic vector bundle provided with a hermitian metric. Using Chern-Weil theory, we can associate to $\overline{E}$ a differential form $\varphi(\overline{E}) = \varphi(-K)$, where K is

the curvature tensor of E viewed as a matrix of 2-forms. The differential form $\varphi(\overline{E})$ is closed and is a sum of components of bidegree (p,p) for $p \geq 0$.
If

$$\overline{\xi}\colon 0 \longrightarrow \overline{E}' \longrightarrow \overline{E} \longrightarrow \overline{E}'' \longrightarrow 0$$

is a short exact sequence of holomorphic vector bundles provided with hermitian metrics, then the differential forms $\varphi(\overline{E})$ and $\varphi(\overline{E}' \oplus \overline{E}')$ may be different, but they represent the same cohomology class.
The Bott-Chern form associated to $\overline{\xi}$ is a solution of the differential equation

$$-2\partial\bar{\partial}\varphi(\overline{\xi}) = \varphi(\overline{E}' \oplus \overline{E}') - \varphi(\overline{E}) \tag{0.1}$$

obtained in a functorial way. The class of a Bott-Chern form modulo the image of ∂ and $\overline{\partial}$ is called a Bott-Chern class and is denoted by $\widetilde{\varphi}(\overline{\xi})$.
There are three ways of defining the Bott-Chern classes. The first one is the original definition of Bott and Chern [7]. It is based on a deformation between the connection associated to $\overline{E}$ and the connection associated to $\overline{E}' \oplus \overline{E}''$. This deformation is parameterized by a real variable.
In [17] Gillet and Soulé introduced a second definition of Bott-Chern classes that is based on a deformation between $\overline{E}$ and $\overline{E}' \oplus \overline{E}''$ parameterized by a projective line. This second definition is used in [4] to prove that the Bott-Chern classes are characterized by three properties

(i) The differential equation (0.1).

(ii) Functoriality (i.e. compatibility with pull-backs via holomorphic maps).

(iii) The vanishing of the Bott-Chern class of a orthogonally split exact sequence.

In [4] Bismut, Gillet and Soulé have a third definition of Bott-Chern classes based on the theory of superconnections. This definition is useful to link Bott-Chern classes with analytic torsion forms.
The definition of Bott-Chern classes can be generalized to any bounded exact sequence of hermitian vector bundles (see section 2 for details). Let

$$\overline{\xi}\colon 0 \longrightarrow (E_n,h_n) \longrightarrow \dots \longrightarrow (E_1,h_1) \longrightarrow (E_0,h_0) \longrightarrow 0$$

be a bounded acyclic complex of hermitian vector bundles; by this we mean a bounded acyclic complex of vector bundles, where each vector bundle is equipped with an arbitrarily chosen hermitian metric. Let

$$r = \sum_{i \text{ even}} \operatorname{rk}(E_i) = \sum_{i \text{ odd}} \operatorname{rk}(E_i).$$

As before, let φ be a symmetric power series in r variables. A Bott-Chern class associated to $\overline{\xi}$ satisfies the differential equation

$$-2\partial\bar{\partial}\widetilde{\varphi}(\overline{\xi}) = \varphi(\bigoplus_k \overline{E}_{2k}) - \varphi(\bigoplus_k \overline{E}_{2k+1}).$$

In particular, let "ch" denote the power series associated to the Chern character class. The Chern character class has the advantage of being additive for direct sums. Then, the Bott-Chern class associated to the long exact sequence $\overline{\xi}$ and to the Chern character class satisfies the differential equation

$$-2\partial\bar{\partial}\widetilde{\mathrm{ch}}(\overline{\xi}) = -\sum_{k=0}^{n}(-1)^i \mathrm{ch}(\overline{E}_k).$$

Let now $i\colon Y \longrightarrow X$ be a closed immersion of complex manifolds. Let $\overline{F}$ be a holomorphic vector bundle on Y provided with a hermitian metric. Let $\overline{N}$ be the normal bundle to Y in X provided also with a hermitian metric. Let

$$0 \longrightarrow \overline{E}_n \longrightarrow \overline{E}_{n-1} \longrightarrow \dots \longrightarrow \overline{E}_0 \longrightarrow i_*F \longrightarrow 0$$

be a resolution of the coherent sheaf i_*F by locally free sheaves, provided with hermitian metrics (following Zha [32] we shall call such a sequence a metric on the coherent sheaf i_*F). Let Td denote the Todd characteristic class. Then the Grothendieck-Riemann-Roch theorem for the closed immersion i implies that the current $i_*(\mathrm{Td}(\overline{N})^{-1}\mathrm{ch}(\overline{F}))$ and the differential form $\sum_k(-1)^k \mathrm{ch}(\overline{E}_k)$ represent the same class in cohomology. We denote $\overline{\xi}$ the data consisting in the closed embedding i, the hermitian bundle $\overline{N}$, the hermitian bundle $\overline{F}$ and the resolution $\overline{E}_* \longrightarrow i_*F$.

In the paper [5], Bismut, Gillet and Soulé introduced a current associated to the above situation. These currents are called singular Bott-Chern currents and denoted in [5] by $T(\overline{\xi})$. When the hermitian metrics satisfy a certain technical condition (condition A of Bismut) then the singular Bott-Chern current $T(\overline{\xi})$ satisfies the differential equation

$$-2\partial\bar{\partial}T(\overline{\xi}) = i_*(\mathrm{Td}(\overline{N})^{-1}\mathrm{ch}(\overline{F})) - \sum_{i=0}^{n}(-1)^i \mathrm{ch}(\overline{E}_i).$$

These singular Bott-Chern currents are among the main ingredients of the proof of Gillet and Soulé's arithmetic Riemann-Roch theorem. In fact it is the main ingredient of the arithmetic Riemann-Roch theorem for closed immersions [6]. This definition of singular Bott-Chern classes is based on the formalism of superconnections, like the third definition of ordinary Bott-Chern classes.

In his thesis [32], Zha gave another definition of singular Bott-Chern currents and used it to give a proof of a different version of the arithmetic Riemann-Roch theorem. This second definition is analogous to Bott and Chern's original definition. Nevertheless there is no explicit comparison between the two definitions of singular Bott-Chern currents.

One of the purposes of this note is to give a third construction of singular Bott-Chern currents, in fact of their classes modulo the image of ∂ and $\overline{\partial}$, which could be seen as analogous to the second definition of Bott-Chern classes. Moreover we will use this third construction to give an axiomatic definition of a theory of singular Bott-Chern classes. A theory of singular Bott-Chern classes is an assignment that, to each data $\overline{\xi}$ as above, associates a class of currents $T(\overline{\xi})$, that satisfies the analogue of conditions (i), (ii) and (iii). The main technical point of this axiomatic definition is that the conditions analogous to (i), (ii) and (iii) above are not enough to characterize the singular Bott-Chern classes. Thus we are led to the problem of classifying the possible theories of Bott-Chern classes, which is the other purpose of this paper.

We fix a theory T of singular Bott-Chern classes. Let Y be a complex manifold and let $\overline{N}$ and $\overline{F}$ be two hermitian holomorphic vector bundles on Y. We write $P = \mathbb{P}(N \oplus 1)$ for the projective completion of N. Let $s\colon Y \longrightarrow P$ be the inclusion as the zero section and let $\pi_P\colon P \longrightarrow Y$ be the projection. Let $\overline{K}_*$ be the Koszul resolution of $s_*\mathcal{O}_Y$ endowed with the metric induced by $\overline{N}$. Then we have a resolution by hermitian vector bundles

$$K(\overline{F},\overline{N})\colon \overline{K}_* \otimes \pi_P^*\overline{F} \longrightarrow s_*F.$$

To these data we associate a singular Bott-Chern class $T(K(\overline{F},\overline{N}))$. It turns out that the current

$$\frac{1}{(2\pi i)^{\operatorname{rk} N}} \int_{\pi_P} T(K(\overline{F},\overline{N})) = (\pi_P)_* T(K(\overline{F},\overline{N}))$$

is closed (see section 3 for general properties of the Bott-Chern classes that imply this property) and determines a characteristic class $C_T(F,N)$ on Y for the vector bundles N and F. Conversely, any arbitrary characteristic class for pairs of vector bundles can be obtained in this way. This allows us to classify the possible theories of singular Bott-Chern classes:

Claim (theorem 7.1). The assignment that sends a singular Bott-Chern class T to the characteristic class C_T is a bijection between the set of theories of singular Bott-Chern classes and the set of characteristic classes.

The next objective of this note is to study the properties of the different theories of singular Bott-Chern classes and of the corresponding characteristic classes. We mention, in the first place, that for the functoriality condition to make sense, we have to study the wave front sets of the currents representing the singular Bott-Chern classes. In particular we use a Poincaré Lemma for currents with fixed wave front set. This result implies that, in each singular Bott-Chern class, we can find a representative with controlled wave front set that can be pulled back with respect certain morphisms.

We also investigate how different properties of the singular Bott-Chern classes T are reflected in properties of the characteristic classes C_T. We thus characterize the compatibility of the singular Bott-Chern classes with the projection formula, by the property of C_T of being compatible with the projection formula. We also relate the compatibility of the singular Bott-Chern classes with the composition of successive closed immersions to an additivity property of the associated characteristic class.

Furthermore, we show that we can add a natural fourth axiom to the conditions analogue to (i), (ii) and (iii), namely the condition of being homogeneous (see section 9 for the precise definition).

Claim (theorem 9.11). There exists a unique homogeneous theory of singular Bott-Chern classes.

Thanks to this axiomatic characterization, we prove that this theory agrees with the theories of singular Bott-Chern classes introduced by Bismut, Gillet and Soulé [6], and by Zha [32]. In particular this provides us a comparison between the two definitions. We will also characterize the characteristic class C_{T^h} for the theory of homogeneous singular Bott-Chern classes.
The last objective of this paper is to give a proof of the arithmetic Riemann-Roch theorem for closed immersions. A version of this theorem was proved by Bismut, Gillet and Soulé and by Zha.
Next we will discuss the contents of the different sections of this paper. In section §1 we recall the properties of characteristic classes in analytic Deligne cohomology. A characteristic class is just a functorial assignment that associates a cohomology class to each vector bundle. The main result of this section is that any characteristic class is given by a power series on the Chern classes, with appropriate coefficients.
In section §2 we recall the theory of Bott-Chern forms and its main properties. The contents of this section are standard although the presentation is slightly different to the ones published in the literature.
In section §3 we study certain direct images of Bott-Chern forms. The main result of this section is that, even if the Bott-Chern classes are not closed, certain direct images of Bott-Chern classes are closed. This result generalizes previous results of Bismut, Gillet and Soulé and of Mourougane. This result is used to prove that the class C_T mentioned previously is indeed a cohomology class, but it can be of independent interest because it implies that several identities in characteristic classes are valid at the level of differential forms.
In section §4 we study the cohomology of the complex of currents with a fixed wave front set. The main result of this section is a Poincaré lemma for currents of this kind. This implies in particular a $\partial\bar{\partial}$-lemma. The results of this section are necessary to state the functorial properties of singular Bott-Chern classes.
In section §5 we recall the deformation of resolutions, that is a generalization of the deformation to the normal cone, and we also recall the construction of the Koszul resolution. These are the main geometric tools used to study singular Bott-Chern classes.
Sections §6 to §9 are devoted to the definition and study of the theories of singular Bott-Chern classes. Section §6 contains the definition and first properties. Section §7 is devoted to the classification theorem of such theories. In section §8 we study how properties of the theory of singular Bott-Chern classes and of the associated characteristic class are related. And in section §9 we define the theory of homogeneous singular Bott-Chern classes and we prove that it agrees with the theories defined by Bismut, Gillet and Soulé and by Zha.

Finally in section §10 we define arithmetic K-groups associated to a $\mathcal{D}_{\log}$-arithmetic variety $(\mathcal{X},\mathcal{C})$ (in the sense of [13]) and push-forward maps for closed immersions of metrized arithmetic varieties, at the level of the arithmetic K-groups. After studying the compatibility of these maps with the projection formula and with the push-forward map at the level of currents, we prove a general Riemann-Roch theorem for closed immersions (theorem 10.28) that compares the direct images in the arithmetic K-groups with the direct images in the arithmetic Chow groups. This theorem is compatible, if we choose the theory of homogeneous singular Bott-Chern classes, with the arithmetic Riemann-Roch theorem for closed immersions proved by Bismut, Gillet and Soulé [6] and it agrees with the theorem proved by Zha [32]. Theorem 10.28, together with the arithmetic Grothendieck-Riemann-Roch theorem for submersions proved in [16], can be used to obtain an arithmetic Grothendieck-Riemann-Roch theorem for projective morphisms of regular arithmetic varieties.

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1 Characteristic classes in analytic Deligne cohomology

A characteristic class for complex vector bundles is a functorial assignment which, to each complex continuous vector bundle on a paracompact topological space X, assigns a class in a suitable cohomology theory of X. For example, if the cohomology theory is singular cohomology, it is well known that each characteristic class can be expressed as a power series in the Chern classes. This can be seen for instance, showing that continuous complex vector bundles on a paracompact space X can be classified by homotopy classes of maps from X to the classifying space $BGL_\infty(\mathbb{C})$ and that the cohomology of $BGL_\infty(\mathbb{C})$ is generated by the Chern classes (see for instance [28]).

The aim of this section is to show that a similar result is true if we restrict the class of spaces to the class of quasi-projective smooth complex manifolds, the class of maps to the class of algebraic maps and the class of vector bundles to the class of algebraic vector bundles and we choose analytic Deligne cohomology as our cohomology theory.

This result and the techniques used to prove it are standard. We will use the splitting principle to reduce to the case of line bundles and will then use the projective spaces as a model of the classifying space $BGL_1(\mathbb{C})$. In this section we also recall the definition of Chern classes in analytic Deligne cohomology and we fix some notations that will be used through the paper.

Definition 1.1. Let X be a complex manifold. For each integer p, *the analytic real Deligne complex* of X is

$$\mathbb{R}_{X,\mathcal{D}}(p) = (\underline{\mathbb{R}}(p) \longrightarrow \mathcal{O}_X \longrightarrow \Omega^1_X \longrightarrow \dots \longrightarrow \Omega^{p-1}_X) \cong s(\underline{\mathbb{R}}(p) \oplus F^p\Omega^*_X \longrightarrow \Omega^*_X),$$

where $\underline{\mathbb{R}}(p)$ is the constant sheaf $(2\pi i)^p\mathbb{R} \subseteq \underline{\mathbb{C}}$. The *analytic real Deligne cohomology of* X, denoted $H^*_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(p))$, is the hyper-cohomology of the above complex.

Analytic Deligne cohomology satisfies the following result.

Theorem 1.2. *The assignment* $X \longmapsto H^*_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(*)) = \bigoplus_p H^*_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(p))$ *is a contravariant functor between the category of complex manifolds and holomorphic maps and the category of unitary bigraded rings that are graded commutative (with respect to the first degree) and associative. Moreover there exists a functorial map*

$$c\colon \operatorname{Pic}(X) = H^1(X, \mathcal{O}^*_X) \longrightarrow H^2_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(1))$$

and, for each closed immersion of complex manifolds $i\colon Y \longrightarrow X$ *of codimension* p*, there exists a morphism*

$$i_*\colon H^*_{\mathcal{D}^{\mathrm{an}}}(Y, \mathbb{R}(*)) \longrightarrow H^{*+2p}_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(* + p))$$

satisfying the properties

A1 Let X *be a complex manifold and let* E *be a holomorphic vector bundle of rank* r*. Let* $\mathbb{P}(E)$ *be the associated projective bundle and let* $\mathcal{O}(-1)$ *the tautological line bundle. The map*

$$\pi^*\colon H^*_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(*)) \longrightarrow H^*_{\mathcal{D}^{\mathrm{an}}}(\mathbb{P}(E), \mathbb{R}(*))$$

induced by the projection $\pi\colon \mathbb{P}(E) \longrightarrow X$ *gives to the second ring a structure of left module over the first. Then the elements* $c(\mathrm{cl}(\mathcal{O}(-1)))^i$*,* $i = 0, \dots, r-1$ *form a basis of this module.*

A2 If X *is a complex manifold,* L *a line bundle,* s *a holomorphic section of* L *that is transverse to the zero section,* Y *is the zero locus of* s *and* $i\colon Y \longrightarrow X$ *the inclusion, then*

$$c(\mathrm{cl}(L)) = i_*(1_Y).$$

A3 If $j\colon Z \longrightarrow Y$ *and* $i\colon Y \longrightarrow X$ *are closed immersions of complex manifolds then* $(ij)_* = i_*j_*$.

A4 If $i\colon Y \longrightarrow X$ is a closed immersion of complex manifolds then, for every $a \in H^{*}_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(*))$ and $b \in H^{*}_{\mathcal{D}^{\mathrm{an}}}(Y, \mathbb{R}(*))$

$$i_{*}(bi^{*}a) = (i_{*}b)a.$$

Proof. The functoriality is clear. The product structure is described, for instance, in [15]. The morphism c is defined by the morphism in the derived category

$$\mathcal{O}_X^{*}[1] \xleftarrow{\cong} s(\underline{\mathbb{Z}}(1) \to \mathcal{O}_X) \longrightarrow s(\underline{\mathbb{R}}(1) \to \mathcal{O}_X) = \mathbb{R}_{\mathcal{D}}(1).$$

The morphism i_{*} can be constructed by resolving the sheaves $\mathbb{R}_{\mathcal{D}}(p)$ by means of currents (see [26] for a related construction). Properties A3 and A4 follow easily from this construction.

By abuse of notation, we will denote by $c_1(\mathcal{O}(-1))$ the first Chern class of $\mathcal{O}(-1)$ with the algebro-geometric twist, in any of the groups $H^2(\mathbb{P}(E), \underline{\mathbb{R}}(1))$, $H^2(\mathbb{P}(E), \underline{\mathbb{C}})$, $H^1(\mathbb{P}(E), \Omega^1_{\mathbb{P}(E)})$. Then, we have sheaf isomorphisms (see for instance [22] for a related result),

$$\bigoplus_{i=0}^{r-1} \underline{\mathbb{R}}_X(p-i)[-2i] \longrightarrow R\pi_{*}\underline{\mathbb{R}}_{\mathbb{P}(E)}(p)$$

$$\bigoplus_{i=0}^{r-1} \Omega^{*}_X[-2i] \longrightarrow R\pi_{*}\Omega^{*}_{\mathbb{P}(E)}$$

$$\bigoplus_{i=0}^{r-1} F^{p-i}\Omega^{*}_X[-2i] \longrightarrow R\pi_{*}F^{p}\Omega^{*}_{\mathbb{P}(E)}$$

given, all of them, by $(a_0, \dots, a_{r-1}) \longmapsto \sum a_i c_1(\mathcal{O}(-1))^i$. Hence we obtain a sheaf isomorphism

$$\bigoplus_{i=0}^{r-1} \mathbb{R}_{X,\mathcal{D}}(p-i)[-2i] \longrightarrow R\pi_{*}\mathbb{R}_{\mathbb{P}(E),\mathcal{D}}(p)$$

from which property A1 follows. Finally property A2 in this context is given by the Poincare-Lelong formula (see [13] proposition 5.64). □

Notation 1.3. For the convenience of the reader, we gather here together several notations and conventions regarding the differential forms, currents and Deligne cohomology that will be used through the paper.

Throughout this paper we will use consistently the algebro-geometric twist. In particular the Chern classes c_i, $i = 0, \dots$ in Betti cohomology will live in $c_i \in H^{2i}(X, \mathbb{R}(i))$; hence our normalizations differ from the ones in [18] where real forms and currents are used.

Moreover we will use the following notations. We will denote by $\mathscr{E}^{*}_X$ the sheaf of Dolbeault algebras of differential forms on X and by $\mathscr{D}^{*}_X$ the sheaf of Dolbeault complexes of currents on X (see [13] §5.4 for the structure of Dolbeault complex of $\mathscr{D}^*_X$). We will denote by $E^*(X)$ and by $D^*(X)$ the complexes of global sections of $\mathscr{E}^*_X$ and $\mathscr{D}^*_X$ respectively. Following [9] and [13] definition 5.10, we denote by $(\mathcal{D}^*(\_,*), \mathrm{d}_{\mathcal{D}})$ the functor that associates to a Dolbeault complex its corresponding Deligne complex. For shorthand, we will denote

$$\mathcal{D}^*(X,p) = \mathcal{D}^*(E^*(X),p),$$
$$\mathcal{D}^*_D(X,p) = \mathcal{D}^*(D^*(X),p).$$

To keep track of the algebro-geometric twist we will use the conventions of [13] §5.4 regarding the current associated to a locally integrable differential form

$$[\omega](\eta) = \frac{1}{(2\pi i)^{\dim X}} \int_X \eta \wedge \omega$$

and the current associated with a subvariety Y

$$\delta_Y(\eta) = \frac{1}{(2\pi i)^{\dim Y}} \int_Y \eta.$$

With these conventions, we have a bigraded morphism $\mathcal{D}^*(X,*) \to \mathcal{D}^*_D(X,*)$ and, if Y has codimension p, the current δ_Y belongs to $\mathcal{D}^{2p}_D(X,p)$. Then $\mathcal{D}^*(X,p)$ and $\mathcal{D}^*_D(X,p)$ are the complex of global sections of an acyclic resolution of $\mathbb{R}_{X,\mathcal{D}}(p)$. Therefore

$$H^*_{\mathcal{D}^{\mathrm{an}}}(X,\mathbb{R}(p)) = H^*(\mathcal{D}(X,p)) = H^*(\mathcal{D}_D(X,p)).$$

If $f : X \to Y$ is a proper smooth morphism of complex manifolds of relative dimension e, then the integral along the fibre morphism

$$f_* : \mathcal{D}^k(X,p) \longrightarrow \mathcal{D}^{k-2e}(X,p-e)$$

is given by

$$f_*\omega = \frac{1}{(2\pi i)^e} \int_f \omega. \tag{1.4}$$

If $(\mathcal{D}^*(*), \mathrm{d}_{\mathcal{D}})$ is a Deligne complex associated to a Dolbeault complex, we will write

$$\widetilde{\mathcal{D}}^k(X,p) := \mathcal{D}^k(X,p)/\,\mathrm{d}_{\mathcal{D}}\,\mathcal{D}^{k-1}(X,p).$$

Finally, following [13] 5.14 we denote by $\bullet$ the product in the Deligne complex that induces the usual product in Deligne cohomology. Note that, if $\omega \in \bigoplus_p \mathcal{D}^{2p}(X,p)$, then for any $\eta \in \mathcal{D}^*(X,*)$ we have $\omega \bullet \eta = \eta \bullet \omega = \eta \wedge \omega$. Sometimes, in this case we will just write $\eta\omega := \eta \bullet \omega$.

We denote by $*$ the complex manifold consisting on one single point. Then

$$H^n_{\mathcal{D}^{\mathrm{an}}}(*,p) = \begin{cases} \mathbb{R}(p) := (2\pi i)^p\mathbb{R}, & \text{if } n=0,\ p \leq 0,\\ \mathbb{R}(p-1) := (2\pi i)^{p-1}\mathbb{R}, & \text{if } n=1,\ p>0.\\ \{0\}, & \text{otherwise.}\end{cases}$$

The product structure in this case is the bigraded product that is given by complex number multiplication when the degrees allow the product to be non zero. We will denote by $\mathbb{D}$ this ring. This is the base ring for analytic Deligne cohomology. Note that, in particular, $H^1_{\mathcal{D}^{\mathrm{an}}}(*,1) = \mathbb{R} = \mathbb{C}/\mathbb{R}(1)$. We will denote by $\mathbf{1}_1$ the image of 1 in $H^1_{\mathcal{D}^{\mathrm{an}}}(*,1)$.
Following [23], theorem 1.2 implies the existence of a theory of Chern classes for holomorphic vector bundles in analytic Deligne cohomology. That is, to every vector bundle E, we can associate a collection of Chern classes $c_i(E) \in H^{2i}_{\mathcal{D}^{\mathrm{an}}}(X,\mathbb{R}(i))$, $i \geq 1$ in a functorial way.
We want to see that all possible characteristic classes in analytic Deligne cohomology can be derived from the Chern classes.

Definition 1.5. Let $n \geq 1$ be an integer and let $r_1 \geq 1, \dots, r_n \geq 1$ be a collection of integers. A *theory of characteristic classes for n-tuples of vector bundles of rank* $r_1, \dots, r_n$ is an assignment that, to each n-tuple of isomorphism classes of vector bundles $(E_1, \dots, E_n)$ over a complex manifold X, with $\mathrm{rk}(E_i) = r_i$, assigns a class

$$\mathrm{cl}(E_1, \dots, E_n) \in \bigoplus_{k,p} H^k_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(p))$$

in a functorial way. That is, for every morphism $f\colon X \longrightarrow Y$ of complex manifolds, the equality

$$f^*(\mathrm{cl}(E_1, \dots, E_n)) = \mathrm{cl}(f^*E_1, \dots, f^*E_n)$$

holds

The first consequence of the functoriality and certain homotopy property of analytic Deligne cohomology classes is the following.

Proposition 1.6. *Let* cl *be a theory of characteristic classes for n-tuples of vector bundles of rank $r_1, \dots, r_n$. Let X be a complex manifold and let $(E_1, \dots, E_n)$ be a n-tuple of vector bundles over X with* $\mathrm{rk}(E_i) = r_i$ *for all i. Let $1 \leq j \leq n$ and let*

$$0 \longrightarrow E'_j \longrightarrow E_j \longrightarrow E''_j \longrightarrow 0,$$

be a short exact sequence. Then the equality

$$\mathrm{cl}(E_1, \dots, E_j, \dots, E_n) = \mathrm{cl}(E_1, \dots, E'_j \oplus E''_j, \dots, E_n)$$

holds.

Proof. Let $\iota_0, \iota_\infty \colon X \longrightarrow X \times \mathbb{P}^1$ be the inclusion as the fiber over 0 and the fiber over ∞ respectively. Then there exists a vector bundle $\widetilde{E}_j$ on $X \times \mathbb{P}^1$ (see for instance [19] (1.2.3.1) or definition 2.5 below) such that $\iota_0^*\widetilde{E}_j \cong E_j$ and $\iota_\infty^*\widetilde{E}_j \cong E'_j \oplus E''_j$. Let $p_1\colon X \times \mathbb{P}^1 \longrightarrow X$ be the first projection. Let $\omega \in \bigoplus_{k,p} \mathcal{D}^k(X,p)$ be any $\mathrm{d}_{\mathcal{D}}$-closed form that represents

$\mathrm{cl}(p_1^*E_1,\dots,\widetilde{E}_j,\dots,p_1^*E_n)$. Then, by functoriality we know that $\iota_0^*\omega$ represents $\mathrm{cl}(E_1,\dots,E_j,\dots,E_n)$ and $\iota_\infty^*\omega$ represents $\mathrm{cl}(E_1,\dots,E_j'\oplus E_j'',\dots,E_n)$. We write

$$\beta=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log t\bar{t}\bullet\omega,$$

where t is the absolute coordinate of $\mathbb{P}^1$. Then

$$\mathrm{d}_{\mathcal{D}}\,\beta=\iota_\infty^*\omega-\iota_0^*\omega$$

which implies the result. □

A standard method to produce characteristic classes for vector bundles is to choose hermitian metrics on the vector bundles and to construct closed differential forms out of them. The following result shows that functoriality implies that the cohomology classes represented by these forms are independent from the hermitian metrics and therefore are characteristic classes. When working with hermitian vector bundles we will use the convention that, if E denotes the vector bundle, then $\overline{E}=(E,h)$ will denote the vector bundle together with the hermitian metric.

Proposition 1.7. *Let $n\geq 1$ be an integer and let $r_1\geq 1,\dots,r_n\geq 1$ be a collection of integers. Let* cl *be an assignment that, to each n-tuple $(\overline{E}_1,\dots,\overline{E}_n)=((E_1,h_1),\dots,(E_n,h_n))$ of isometry classes of hermitian vector bundles of rank $r_1,\dots,r_n$ over a complex manifold X, associates a cohomology class*

$$\mathrm{cl}(\overline{E}_1,\dots,\overline{E}_n)\in\bigoplus_{k,p}H^k_{\mathcal{D}}(X,\mathbb{R}(p))$$

such that, for each morphism $f:Y\to X$,

$$\mathrm{cl}(f^*\overline{E}_1,\dots,f^*\overline{E}_n)=f^*\,\mathrm{cl}(\overline{E}_1,\dots,\overline{E}_n).$$

Then the cohomology class $\mathrm{cl}(\overline{E}_1,\dots,\overline{E}_n)$ is independent from the hermitian metrics. Therefore it is a well defined characteristic class.

Proof. Let $1\leq j\leq n$ be an integer and let $\overline{E}_j'=(E_j,h_j')$ be the vector bundle underlying $\overline{E}_j$ with a different choice of metric. Let ι_0, ι_∞ and p_1 be as in the proof of proposition 1.6. Then we can choose a hermitian metric h on $p_1^*E_j$, such that $\iota_0^*(p_1^*E_j,h)=\overline{E}_j$ and $\iota_\infty^*(p_1^*E_j,h)=\overline{E}_j'$. Let ω be any smooth closed differential form on $X\times\mathbb{P}^1$ that represents $\mathrm{cl}(p_1^*\overline{E}_1,\dots,(p_1^*E_1,h),\dots,p_1^*\overline{E}_n)$. Then,

$$\beta=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log t\bar{t}\bullet\omega$$

satisfies

$$\mathrm{d}_{\mathcal{D}}\,\beta=\iota_\infty^*\omega-\iota_0^*\omega$$

which implies the result. □

We are interested in vector bundles that can be extended to a projective variety. Therefore we will restrict ourselves to the algebraic category. So, by a complex algebraic manifold we will mean the complex manifold associated to a smooth quasi-projective variety over $\mathbb{C}$. When working with an algebraic manifold, by a vector bundle we will mean the holomorphic vector bundle associated to an algebraic vector bundle.
We will denote by $\mathbb{D}[[x_1,\dots,x_r]]$ the ring of commutative formal power series. That is, the unknowns $x_1,\dots,x_r$ commute with each other and with $\mathbb{D}$. We turn it into a commutative bigraded ring by declaring that the unknowns x_i have bidegree $(2,1)$. The symmetric group in r elements, $\mathfrak{S}_r$ acts on $\mathbb{D}[[x_1,\dots,x_r]]$. The subalgebra of invariant elements is generated over $\mathbb{D}$ by the elementary symmetric functions. The main result of this section is the following

Theorem 1.8. *Let* cl *be a theory of characteristic classes for n-tuples of vector bundles of rank $r_1,\dots,r_n$. Then, there is a power series $\varphi\in\mathbb{D}[[x_1,\dots,x_r]]$ in $r=r_1+\dots+r_n$ variables with coefficients in the ring $\mathbb{D}$, such that, for each complex algebraic manifold X and each n-tuple of algebraic vector bundles $(E_1,\dots,E_n)$ over X with $\operatorname{rk}(E_i)=r_i$ this equality holds:*

$$\operatorname{cl}(E_1,\dots,E_n)=\varphi(c_1(E_1),\dots,c_{r_1}(E_1),\dots,c_1(E_n),\dots,c_{r_n}(E_n)). \tag{1.9}$$

Conversely, any power series φ as before determines a theory of characteristic classes for n-tuples of vector bundles of rank $r_1,\dots,r_n$, by equation (1.9)*.*

Proof. The second statement is obvious from the properties of Chern classes. Since we are assuming X quasi-projective, given n algebraic vector bundles $E_1,\dots,E_n$ on X, there is a smooth projective compactification $\widetilde{X}$ and vector bundles $\widetilde{E}_1,\dots,\widetilde{E}_n$ on $\widetilde{X}$, such that $E_i=\widetilde{E}_i|_X$ (see for instance [14] proposition 2.2), we are reduced to the case when X is projective. In this case, analytic Deligne cohomology agrees with ordinary Deligne cohomology.
Let us assume first that $r_1=\dots=r_n=1$ and that we have a characteristic class cl for n line bundles. Then, for each n-tuple of positive integers $m_1,\dots,m_n$ we consider the space $\mathbb{P}^{m_1,\dots,m_n}=\mathbb{P}^{m_1}_{\mathbb{C}}\times\dots\times\mathbb{P}^{m_n}_{\mathbb{C}}$ and we denote by p_i the projection over the i-th factor. Then

$$\bigoplus_{k,p}H^k_{\mathcal{D}}(\mathbb{P}^{m_1,\dots,m_n},\mathbb{R}(p))=\mathbb{D}[x_1,\dots,x_n]\Big/(x_1^{m_1},\dots,x_n^{m_n})$$

is a quotient of the polynomial ring generated by the classes $x_i=c_1(p_i^*\mathcal{O}(1))$ with coefficients in the ring $\mathbb{D}$. Therefore, there is a polynomial $\varphi_{m_1,\dots,m_n}$ in n variables such that

$$\operatorname{cl}(p_1^*\mathcal{O}(1),\dots,p_1^*\mathcal{O}(1))=\varphi_{m_1,\dots,m_n}(x_1,\dots,x_n).$$

If $m_1\le m_1'$, …, $m_n\le m_n'$ then, by functoriality, the polynomial $\varphi_{m_1,\dots,m_n}$ is the truncation of the polynomial $\varphi_{m_1',\dots,m_n'}$. Therefore there is a power series

in n variables, φ such that $\varphi_{m_1,\dots,m_n}$ is the truncation of φ in the appropriate quotient of the polynomial ring.
Let $L_1,\dots,L_n$ be line bundles on a projective algebraic manifold that are generated by global sections. Then they determine a morphism $f\colon X \longrightarrow \mathbb{P}^{m_1,\dots,m_n}$ such that $L_i = f^*p_i^*\mathcal{O}(1)$. Therefore, again by functoriality, we obtain

$$\mathrm{cl}(L_1,\dots,L_n) = \varphi(c_1(L_1),\dots,c_1(L_n)).$$

From the class cl we can define a new characteristic class for $n+1$ line bundles by the formula

$$\mathrm{cl}'(L_1,\dots,L_n,M) = \mathrm{cl}(L_1\otimes M^\vee,\dots,L_n\otimes M^\vee).$$

When $L_1,\dots,L_n$ and M are generated by global sections we have that there is a power series ψ such that

$$\mathrm{cl}'(L_1,\dots,L_n,M) = \psi(c_1(L_1),\dots,c_1(L_n),c_1(M)).$$

Moreover, when the line bundles $L_i\otimes M^\vee$ are also generated by global sections the following holds

$$\begin{aligned}\psi(c_1(L_1),\dots,c_1(L_n),c_1(M)) &= \varphi(c_1(L_1\otimes M^\vee),\dots,c_1(L_n\otimes M^\vee))\\ &= \varphi(c_1(L_1)-c_1(M),\dots,c_1(L_n)-c_1(M)).\end{aligned}$$

Considering the system of spaces $\mathbb{P}^{m_1,\dots,m_n,m_{n+1}}$ with line bundles

$$L_i = p_i^*\mathcal{O}(1)\otimes p_{n+1}^*\mathcal{O}(1),\ i=1,\dots,n, \quad M = p_{n+1}^*\mathcal{O}(1),$$

we see that there is an identity of power series

$$\varphi(x_1-y,\dots,x_n-y) = \psi(x_1,\dots,x_n,y).$$

Now let X be a projective complex manifold and let $L_1,\dots,L_n$ be arbitrary line bundles. Then there is a line bundle M such that M and $L_i' = L_i\otimes M$, $i=1,\dots,n$ are generated by global sections. Then we have

$$\begin{aligned}\mathrm{cl}(L_1,\dots,L_n) &= \mathrm{cl}(L_1'\otimes M^\vee,\dots,L_n'\otimes M^\vee)\\ &= \mathrm{cl}'(L_1',\dots,L_n',M)\\ &= \psi(c_1(L_1'),\dots,c_1(L_n'),c_1(M))\\ &= \varphi((c_1(L_1')-c_1(M),\dots,c_1(L_n')-c_1(M)))\\ &= \varphi(c_1(L_1),\dots,c_1(L_n)).\end{aligned}$$

The case of arbitrary rank vector bundles follows from the case of rank one vector bundles by proposition 1.6 and the splitting principle. We next recall the argument. Given a projective complex manifold X and vector bundles $E_1,\dots,E_n$ of rank $r_1,\dots,r_n$, we can find a proper morphism $\pi\colon \widetilde{X} \longrightarrow X$, with $\widetilde{X}$ a complex projective manifold, and such that the induced morphism

$$\pi^*\colon H^*_{\mathcal{D}}(X,\mathbb{R}(*)) \longrightarrow H^*_{\mathcal{D}}(\widetilde{X},\mathbb{R}(*))$$

is injective and every bundle $\pi^*(E_i)$ admits a holomorphic filtration

$$0 = K_{i,0} \subset K_{i,1} \subset \cdots \subset K_{i,r_i-1} \subset K_{i,r_i} = \pi^*(E_i),$$

with $L_{i,j} = K_{i,j}/K_{i,j-1}$ a line bundle. If cl is a characteristic class for n-tuples of vector bundles of rank $r_1, \dots, r_n$, we define a characteristic class for $r_1 + \cdots + r_n$-tuples of line bundles by the formula

$$\mathrm{cl}'(L_{1,1}, \dots, L_{1,r_1}, \dots, L_{n,1}, \dots, L_{n,r_n}) = \mathrm{cl}(L_{1,1} \oplus \cdots \oplus L_{1,r_1}, \dots, L_{n,1} \oplus \cdots \oplus, L_{n,r_n}).$$

By the case of line bundles we know that there is a power series in $r_1 + \cdots + r_n$ variables ψ such that

$$\mathrm{cl}'(L_{1,1}, \dots, L_{1,r_1}, \dots, L_{n,1}, \dots, L_{n,r_n}) = \psi(c_1(L_{1,1}), \dots, c_1(L_{n,r_n})).$$

Since the class cl' is symmetric under the group $\mathfrak{S}_{r_1} \times \cdots \times \mathfrak{S}_{r_n}$, the same is true for the power series ψ. Therefore ψ can be written in terms of symmetric elementary functions. That is, there is another power series in $r_1 + \cdots + r_n$ variables φ, such that

$$\psi(x_{1,1}, \dots, x_{n,r_n}) = \varphi(s_1(x_{1,1}, \dots, x_{1,r_1}), \dots, s_{r_1}(x_{1,1}, \dots, x_{1,r_1}), \dots \\ \dots, s_1(x_{n,1}, \dots, x_{n,r_n}), \dots, s_{r_n}(x_{n,1}, \dots, x_{n,r_n})),$$

where s_i is the i-th elementary symmetric function of the appropriate number of variables. Then

$$\begin{aligned}\pi^*(\mathrm{cl}(E_1, \dots, E_n)) &= \mathrm{cl}(\pi^* E_1, \dots, \pi^* E_n)) \\ &= \mathrm{cl}'(L_{1,1}, \dots, L_{n,r_n}) \\ &= \psi(c_1(L_{1,1}), \dots, c_1(L_{n,r_n})) \\ &= \varphi(c_1(\pi^* E_1), \dots, c_{r_1}(\pi^* E_1), \dots, c_1(\pi^* E_n), \dots, c_{r_n}(\pi^* E_n)) \\ &= \pi^* \varphi(c_1(E_1), \dots, c_{r_1}(E_1), \dots, c_1(E_n), \dots, c_{r_n}(E_n)).\end{aligned}$$

Therefore, the result follows from the injectivity of π^*. □

Remark 1.10. It would be interesting to know if the functoriality of a characteristic class in enough to imply that it is a power series in the Chern classes for arbitrary complex manifolds and holomorphic vector bundles.

2 Bott-Chern classes

The aim of this section is to recall the theory of Bott-Chern classes. For more details we refer the reader to [7], [4], [19], [31], [14], [10] and [12]. Note however that the theory we present here is equivalent, although not identical, to the different versions that appear in the literature.

Let X be a complex manifold and let $\overline{E} = (E, h)$ be a rank r holomorphic vector bundle provided with a hermitian metric. Let $\phi \in \mathbb{D}[[x_1, \dots, x_r]]$ be a formal power series in r variables that is symmetric under the action of $\mathfrak{S}_r$. Let s_i, $i = 1, \dots, r$ be the elementary symmetric functions in r variables. Then $\phi(x_1, \dots, x_r) = \varphi(s_1, \dots, s_r)$ for certain power series φ. By Chern-Weil theory we can obtain a representative of the class

$$\phi(E) := \varphi(c_1(E), \dots, c_r(E)) \in \bigoplus_{k,p} H^k_{\mathcal{D}^{\mathrm{an}}}(X, \mathbb{R}(p))$$

as follows.

We denote also by ϕ the invariant power series in $r \times r$ matrices defined by ϕ. Let K be the curvature matrix of the hermitian holomorphic connection of (E, h). The entries of K in a particular trivialization of E are local sections of $\mathcal{D}^2(X, 1)$. Then we write

$$\phi(E, h) = \phi(-K) \in \bigoplus_{k,p} \mathcal{D}^k(X, p).$$

The form $\phi(E, h)$ is well defined, closed, and it represents the class $\phi(E)$.

Now let

$$\overline{E}_* = (\dots \xrightarrow{f_{n+1}} \overline{E}_n \xrightarrow{f_n} \overline{E}_{n-1} \xrightarrow{f_{n-1}} \dots)$$

be a bounded acyclic complex of hermitian vector bundles; by this we mean a bounded acyclic complex of vector bundles, where each vector bundle is equipped with an arbitrarily chosen hermitian metric.

Write

$$r = \sum_{i \text{ even}} \mathrm{rk}(E_i) = \sum_{i \text{ odd}} \mathrm{rk}(E_i).$$

and let ϕ be a symmetric power series in r variables.

As before, we can define the Chern forms

$$\phi(\bigoplus_{i \text{ even}} (E_i, h_i)) \text{ and } \phi(\bigoplus_{i \text{ odd}} (E_i, h_i)),$$

that represent the Chern classes $\phi(\bigoplus_{i \text{ even}} E_i)$ and $\phi(\bigoplus_{i \text{ odd}} E_i)$. The Chern classes are compatible with respect to exact sequences, that is,

$$\phi(\bigoplus_{i \text{ even}} E_i) = \phi(\bigoplus_{i \text{ odd}} E_i).$$

But, in general, this is not true for the Chern forms. This lack of compatibility with exact sequences on the level of Chern forms is measured by the Bott-Chern classes.

Definition 2.1. Let

$$\overline{E}_* = (\dots \xrightarrow{f_{n+1}} \overline{E}_n \xrightarrow{f_n} \overline{E}_{n-1} \xrightarrow{f_{n-1}} \dots)$$

be an acyclic complex of hermitian vector bundles, we will say that $\overline{E}_*$ is an *orthogonally split complex* of vector bundles if, for any integer n, the exact sequence

$$0 \longrightarrow \operatorname{Ker} f_n \longrightarrow \overline{E}_n \longrightarrow \operatorname{Ker} f_{n-1} \longrightarrow 0$$

is split, there is a splitting section $s_n\colon \operatorname{Ker} f_{n-1} \to E_n$ such that $\overline{E}_n$ is the orthogonal direct sum of $\operatorname{Ker} f_n$ and $\operatorname{Im} s_n$ and the metrics induced in the subbundle $\operatorname{Ker} f_{n-1}$ by the inclusion $\operatorname{Ker} f_{n-1} \subset \overline{E}_{n-1}$ and by the section s_n agree.

Notation 2.2. Let $(x : y)$ be homogeneous coordinates of $\mathbb{P}^1$ and let $t = x/y$ be the absolute coordinate. In order to make certain choices of metrics in a functorial way, we fix once and for all a partition of unity $\{\sigma_0, \sigma_\infty\}$, over $\mathbb{P}^1$ subordinated to the open cover of $\mathbb{P}^1$ given by the open subsets $\{\{|y| > 1/2|x|\}, \{|x| > 1/2|y|\}\}$. As usual we will write $\infty = (1 : 0)$, $0 = (0 : 1)$.

The fundamental result of the theory of Bott-Chern classes is the following theorem (see [7], [4], [19]).

Theorem 2.3. *There is a unique way to attach to each bounded exact complex $\overline{E}_*$ as above, a class $\widetilde{\phi}(\overline{E}_*)$ in*

$$\bigoplus_k \widetilde{\mathcal{D}}^{2k-1}(X,k) = \bigoplus_k \mathcal{D}^{2k-1}(X,k)/\operatorname{Im}(\mathrm{d}_{\mathcal{D}})$$

satisfying the following properties

(i) (Differential equation)

$$\mathrm{d}_{\mathcal{D}}\, \widetilde{\phi}(\overline{E}_*) = \phi(\bigoplus_{i\ even} (E_i, h_i)) - \phi(\bigoplus_{i\ odd} (E_i, h_i)). \tag{2.4}$$

(ii) (Functoriality) $f^*\widetilde{\phi}(\overline{E}_*) = \widetilde{\phi}(f^*\overline{E}_*)$, for every holomorphic map $f\colon X' \longrightarrow X$.

(iii) (Normalization) If $\overline{E}_*$ is orthogonally split, then $\widetilde{\phi}(\overline{E}_*) = 0$.

Proof. We first recall how to prove the uniqueness.
Let $\overline{K}_i = (K_i, g_i)$, where $K_i = \operatorname{Ker} f_i$ and g_i is the metric induced by the inclusion $K_i \subset E_i$. Consider the complex manifold $X \times \mathbb{P}^1$ with projections p_1 and p_2. For every vector bundle F on X we will denote $F(i) = p_1^*F \otimes p_2^*\mathcal{O}_{\mathbb{P}^1}(i)$. Let $\widetilde{C}_* = \widetilde{C}(E_*)_*$ be the complex of vector bundles on $X \times \mathbb{P}^1$ given by $\widetilde{C}_i = E_i(i) \oplus E_{i-1}(i-1)$ with differential $d(s,t) = (t,0)$. Let $\widetilde{D}_* = \widetilde{D}(E_*)_*$ be the complex of vector bundles with $\widetilde{D}_i = E_{i-1}(i) \oplus E_{i-2}(i-1)$ and differential $d(s,t) = (t,0)$. Using notation 2.2 we define the map $\psi\colon \widetilde{C}(E_*)_i \longrightarrow \widetilde{D}(E_*)_i$ given by $\psi(s,t) = (f_i(s) - t \otimes y, f_{i-1}(t))$. It is a morphism of complexes.

Definition 2.5. The *first transgression exact sequence* of E_* is given by

$$\operatorname{tr}_1(E_*)_* = \operatorname{Ker}\psi.$$

On $X\times \mathbb{A}^1$, the map $p_1^*E_i \longrightarrow \widetilde{C}(E_*)_i$ given by $s\longmapsto (s\otimes y^i, f_i(s)\otimes y^{i-1})$ induces an isomorphism of complexes

$$p_1^*E_* \longrightarrow \operatorname{tr}_1(E_*)_*|_{X\times\mathbb{A}^1}, \tag{2.6}$$

and in particular isomorphisms

$$\operatorname{tr}_1(E_*)_i|_{X\times\{0\}} \cong E_i. \tag{2.7}$$

Moreover, we have isomorphisms

$$\operatorname{tr}_1(E_*)_i|_{X\times\{\infty\}} \cong K_i\oplus K_{i-1}. \tag{2.8}$$

Definition 2.9. We will denote by $\operatorname{tr}_1(\overline{E}_*)_*$ the complex $\operatorname{tr}_1(E_*)_*$ provided with any hermitian metric such that the isomorphisms (2.7) and (2.8) are isometries. If we need a functorial choice of metric, we proceed as follows. On $X\times(\mathbb{P}^1\setminus\{0\})$ we consider the metric induced by $\widetilde{C}$ on $\operatorname{tr}_1(E_*)_*$. On $X\times(\mathbb{P}^1\setminus\{\infty\})$ we consider the metric induced by the isomorphism (2.6). We glue both metrics by means of the partition of unity of notation 2.2.

In particular, we have that $\operatorname{tr}_1(\overline{E}_*)|_{X\times\{\infty\}}$ is orthogonally split. We assume that there exists a theory of Bott-Chern classes satisfying the above properties. Thus, there exists a class of differential forms $\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)$ with the following properties. By (i) this class satisfies

$$\mathrm{d}_{\mathcal{D}}\,\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)=\phi(\bigoplus_{i\text{ even}}\operatorname{tr}_1(\overline{E}_*)_i))-\phi(\bigoplus_{i\text{ odd}}\operatorname{tr}_1(\overline{E}_*)_i).$$

By (ii), it satisfies

$$\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)\,|_{X\times\{0\}}=\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*\,|_{X\times\{0\}})=\widetilde{\phi}(\overline{E}_*).$$

Finally, by (ii) and (iii) it satisfies

$$\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)\,|_{X\times\{\infty\}}=\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*\,|_{X\times\{\infty\}})=0.$$

Let $\phi(\operatorname{tr}_1(\overline{E}_*)_*)$ be any representative of the class $\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)$.
Then, in the group $\bigoplus_k \widetilde{\mathcal{D}}^{2k-1}(X,k)$, we have

$$\begin{aligned}
0&=\mathrm{d}_{\mathcal{D}}\,\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar t)\bullet\phi(\operatorname{tr}_1(\overline{E}_*)_*)\\
&=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\left(\mathrm{d}_{\mathcal{D}}\,\frac{-1}{2}\log(t\bar t)\bullet\phi(\operatorname{tr}_1(\overline{E}_*)_*)-\frac{-1}{2}\log(t\bar t)\bullet\mathrm{d}_{\mathcal{D}}\,\phi(\operatorname{tr}_1(\overline{E}_*)_*)\right)\\
&=\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)|_{X\times\{\infty\}}-\widetilde{\phi}(\operatorname{tr}_1(\overline{E}_*)_*)|_{X\times\{0\}}\\
&\quad-\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar t)\bullet(\phi(\bigoplus_{i\text{ even}}\operatorname{tr}_1(\overline{E}_*)_i)-\phi(\bigoplus_{i\text{ odd}}\operatorname{tr}_1(\overline{E}_*)_i))\\
&=-\widetilde{\phi}(\overline{E}_*)-\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar t)\bullet(\phi(\bigoplus_{i\text{ even}}\operatorname{tr}_1(\overline{E}_*)_i)-\phi(\bigoplus_{i\text{ odd}}\operatorname{tr}_1(\overline{E}_*)_i)).
\end{aligned}$$

Hence, if such a theory exists, it should satisfy the formula

$$\widetilde{\phi}(\overline{E}_*)=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar{t})\bullet(\phi(\bigoplus_{i\text{ odd}}\operatorname{tr}_1(\overline{E}_*)_i)-\phi(\bigoplus_{i\text{ even}}\operatorname{tr}_1(\overline{E}_*)_i)). \tag{2.10}$$

Therefore $\widetilde{\phi}(\overline{E}_*)$ is determined by properties (i), (ii) and (iii).
In order to prove the existence of a theory of functorial Bott-Chern forms, we have to see that the right hand side of equation (2.10) is independent from the choice of the metric on $\operatorname{tr}_1(\overline{E}_*)_*$ and that it satisfies the properties (i), (ii) and (iii). For this the reader can follow the proof of [4] theorem 1.29.

□

In view of the proof of theorem 2.3, we can define the Bott-Chern classes as follows.

Definition 2.11. Let

$$\overline{E}_*\colon 0\longrightarrow(E_n,h_n)\longrightarrow\dots\longrightarrow(E_1,h_1)\longrightarrow(E_0,h_0)\longrightarrow 0$$

be a bounded acyclic complex of hermitian vector bundles. Let

$$r=\sum_{i\text{ even}}\operatorname{rk}(E_i)=\sum_{i\text{ odd}}\operatorname{rk}(E_i).$$

Let $\phi\in\mathbb{D}[[x_1,\dots,x_r]]^{\mathfrak{S}_r}$ be a symmetric power series in r variables. Then the *Bott-Chern class* associated to ϕ and $\overline{E}_*$ is the element of $\bigoplus_{k,p}\widetilde{\mathcal{D}}^k(E_X,p)$ given by

$$\widetilde{\phi}(\overline{E_*})=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar{t})\bullet(\phi(\bigoplus_{i\text{ odd}}\operatorname{tr}_1(\overline{E}_*)_i)-\phi(\bigoplus_{i\text{ even}}\operatorname{tr}_1(\overline{E}_*)_i)).$$

The following property is obvious from the definition.

Lemma 2.12. *Let $\overline{E}_*$ be an acyclic complex of hermitian vector bundles. Then, for any integer k,*

$$\widetilde{\phi}(\overline{E}_*[k])=(-1)^k\widetilde{\phi}(\overline{E}_*).$$

□

Particular cases of Bott-Chern classes are obtained when we consider a single vector bundle with two different hermitian metrics or a short exact sequence of vector bundles. Note however that, in order to fix the sign of the Bott-Chern classes on these cases, one has to choose the degree of the vector bundles involved, for instance as in the next definition.

Definition 2.13. Let E be a holomorphic vector bundle of rank r, let h_0 and h_1 be two hermitian metrics and let ϕ be an invariant power series of r variables. We will denote by $\widetilde{\phi}(E,h_0,h_1)$ the Bott-Chern class associated to the complex

$$\overline{\xi}\colon 0\longrightarrow(E,h_1)\longrightarrow(E,h_0)\longrightarrow 0,$$

where (E,h_0) sits in degree zero.

Therefore, this class satisfies

$$\mathrm{d}_{\mathcal{D}}\,\widetilde{\phi}(E,h_0,h_1)=\phi(E,h_0)-\phi(E,h_1).$$

In fact we can characterize $\widetilde{\phi}(E,h_0,h_1)$ axiomatically as follows.

Proposition 2.14. *Given ϕ, a symmetric power series in r variables, there is a unique way to attach, to each rank r vector bundle E on a complex manifold X and metrics h_0 and h_1, a class $\widetilde{\phi}(E,h_0,h_1)$ satisfying*

(i) $\mathrm{d}_{\mathcal{D}}\,\widetilde{\phi}(E,h_0,h_1)=\phi(E,h_0)-\phi(E,h_1)$.

(ii) $f^*\widetilde{\phi}(E,h_0,h_1)=\widetilde{\phi}(f^*(E,h_0,h_1))$ *for every holomorphic map* $f\colon Y\longrightarrow X$.

(iii) $\widetilde{\phi}(E,h,h)=0$.

Moreover, if we denote $\widetilde{E}:=\mathrm{tr}_1(\overline{\xi})_1$, *then it satisfies*

$$\widetilde{E}|_{X\times\{\infty\}}\cong(E,h_0),\quad \widetilde{E}|_{X\times\{0\}}\cong(E,h_1)$$

and

$$\widetilde{\phi}(E,h_0,h_1)=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar{t})\bullet\phi(\widetilde{E}). \tag{2.15}$$

Proof. The axiomatic characterization is proved as in theorem 2.3. In order to prove equation (2.15), if we follow the notations of the proof of theorem 2.3 we have $K_0=(E,h_0)$ and $K_1=0$. Therefore $\mathrm{tr}_1(\overline{\xi})_0=p_1^*(E,h_0)$, while $\widetilde{E}:=\mathrm{tr}_1(\overline{\xi})_1$ satisfies $\widetilde{E}|_{X\times\{0\}}=(E,h_1)$ and $\widetilde{E}|_{X\times\{\infty\}}=(E,h_0)$. Using the antisymmetry of $\log t\bar{t}$ under the involution $t\mapsto 1/t$ we obtain

$$\widetilde{\phi}(E,h_0,h_1)=\widetilde{\phi}(\overline{\xi})=\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{-1}{2}\log(t\bar{t})\bullet\phi(\widetilde{E}).$$

□

We can also treat the case of short exact sequences. If

$$\overline{\varepsilon}\colon 0\longrightarrow\overline{E}_2\longrightarrow\overline{E}_1\longrightarrow\overline{E}_0\longrightarrow 0$$

is a short exact sequence of hermitian vector bundles, by convention, we will assume that $\overline{E}_0$ sits in degree zero. This fixs the sign of $\widetilde{\phi}(\overline{\varepsilon})$.

Proposition 2.16. *Given ϕ, a symmetric power series in r variables, there is a unique way to attach, to each short exact sequence of hermitian vector bundles on a complex manifold X*

$$\overline{\varepsilon}\colon 0\longrightarrow\overline{E}_2\longrightarrow\overline{E}_1\longrightarrow\overline{E}_0\longrightarrow 0,$$

where $\overline{E}_1$ has rank r, a class $\widetilde{\phi}(\overline{\varepsilon})$ satisfying

(i) $\mathrm{d}_{\mathcal{D}}\,\widetilde{\phi}(\overline{\varepsilon}) = \phi(\overline{E}_0 \oplus \overline{E}_2) - \phi(\overline{E}_1)$.

(ii) $f^*\widetilde{\phi}(\overline{\varepsilon}) = \widetilde{\phi}(f^*(\overline{\epsilon}))$ *for every holomorphic map* $f\colon Y \longrightarrow X$.

(iii) $\widetilde{\phi}(\overline{\varepsilon}) = 0$ *whenever* $\overline{\varepsilon}$ *is orthogonally split.*

□

The following additivity result of Bott-Chern classes will be useful later.

Lemma 2.17. *Let $\overline{A}_{*,*}$ be a bounded exact sequence of bounded exact sequences of hermitian vector bundles. Let*

$$r = \sum_{i,j\ \text{even}} \operatorname{rk}(A_{i,j}) = \sum_{i,j\ \text{odd}} \operatorname{rk}(A_{i,j}) = \sum_{\substack{i\ \text{odd}\\ j\ \text{even}}} \operatorname{rk}(A_{i,j}) = \sum_{\substack{i\ \text{even}\\ j\ \text{odd}}} \operatorname{rk}(A_{i,j}).$$

Let ϕ be a symmetric power series in r variables. Then

$$\widetilde{\phi}(\bigoplus_{k\ \text{even}} \overline{A}_{k,*}) - \widetilde{\phi}(\bigoplus_{k\ \text{odd}} \overline{A}_{k,*}) = \widetilde{\phi}(\bigoplus_{k\ \text{even}} \overline{A}_{*,k}) - \widetilde{\phi}(\bigoplus_{k\ \text{odd}} \overline{A}_{*,k}).$$

Proof. The proof is analogous to the proof of proposition 6.13 and is left to the reader. □

Corollary 2.18. *Let $\overline{A}_{*,*}$ be a bounded double complex of hermitian vector bundles with exact rows, let*

$$r = \sum_{i+j\ \text{even}} \operatorname{rk}(A_{i,j}) = \sum_{i+j\ \text{odd}} \operatorname{rk}(A_{i,j})$$

and let ϕ be a symmetric power series in r variables. Then

$$\widetilde{\phi}(\operatorname{Tot} \overline{A}_{*,*}) = \widetilde{\phi}(\bigoplus_k \overline{A}_{*,k}[-k]).$$

Proof. Let k_0 be an integer such that $\overline{A}_{k,l} = 0$ for $k < k_0$. For any integer n we denote by $\operatorname{Tot}_n = \operatorname{Tot}((\overline{A}_{k,l})_{k\geq n})$ the total complex of the exact complex formed by the rows with index greater or equal than n. Then $\operatorname{Tot}_{k_0} = \operatorname{Tot}(\overline{A}_{*,*})$. For each k there is an exact sequence of complexes

$$0 \longrightarrow \operatorname{Tot}_{k+1} \longrightarrow \operatorname{Tot}_k \oplus \bigoplus_{l<k} \overline{A}_{l,*}[-l] \longrightarrow \bigoplus_{l\leq k} \overline{A}_{l,*}[-l] \longrightarrow 0,$$

which is orthogonally split in each degree. Therefore by lemma 2.17 we obtain

$$\widetilde{\phi}(\operatorname{Tot}_k \oplus \bigoplus_{l<k} \overline{A}_{l,*}[-l]) = \widetilde{\phi}(\operatorname{Tot}_{k-1} \oplus \bigoplus_{l\leq k} \overline{A}_{l,*}[-l]).$$

Hence the result follows by induction. □

A particularly important characteristic class is the Chern character. This class is additive for exact sequences. Specializing lemma 2.17 and corollary 2.18 to the Chern character we obtain

Corollary 2.19. *With the hypothesis of lemma 2.17, the following equality holds:*

$$\sum_k (-1)^k \widetilde{\mathrm{ch}}(\overline{A}_{k,*}) = \sum_k (-1)^k \widetilde{\mathrm{ch}}(\overline{A}_{*,k}) = \widetilde{\mathrm{ch}}(\mathrm{Tot}\,\overline{A}_{*,*}).$$

□

Our next aim is to extend the Bott-Chern classes associated to the Chern character to metrized coherent sheaves. This extension is due to Zha [32], although it is still unpublished.

Definition 2.20. A *metrized coherent sheaf* $\overline{\mathcal{F}}$ on X is a pair $(\mathcal{F}, \overline{E}_* \to \mathcal{F})$ where $\mathcal{F}$ is a coherent sheaf on X and

$$0 \to \overline{E}_n \to \overline{E}_{n-1} \to \cdots \to \overline{E}_0 \to \mathcal{F} \to 0$$

is a finite resolution by hermitian vector bundles of the coherent sheaf $\mathcal{F}$. This resolution is also called the metric of $\overline{\mathcal{F}}$.
If $\overline{E}$ is a hermitian vector bundle, we will also denote by $\overline{E}$ the metrized coherent sheaf $(E, \overline{E} \xrightarrow{\mathrm{id}} E)$.

Note that the coherent sheaf 0 may have non trivial metrics. In fact, any exact sequence of hermitian vector bundles

$$0 \to \overline{A}_n \to \cdots \to \overline{A}_0 \to 0 \to 0$$

can be seen as a metric on 0. It will be denoted $\overline{0}_{A_*}$. A metric on 0 is said to be *orthogonally split* if the exact sequence is orthogonally split.
A morphism of metrized coherent sheaves $\overline{\mathcal{F}}_1 \to \overline{\mathcal{F}}_2$ is just a morphism of sheaves $\mathcal{F}_1 \to \mathcal{F}_2$. A sequence of metrized coherent sheaves

$$\overline{\varepsilon}: \qquad \dots \longrightarrow \overline{\mathcal{F}}_{n+1} \longrightarrow \overline{\mathcal{F}}_n \longrightarrow \overline{\mathcal{F}}_{n-1} \longrightarrow \dots$$

is said to be exact if it is exact as a sequence of coherent sheaves.

Definition 2.21. Let $\overline{\mathcal{F}} = (\mathcal{F}, \overline{E}_* \to \mathcal{F})$ be a metrized coherent sheaf. Then the *Chern character form* associated to $\overline{\mathcal{F}}$ is given by

$$\mathrm{ch}(\overline{\mathcal{F}}) = \sum_i (-1)^i \,\mathrm{ch}(\overline{E}_i).$$

Definition 2.22. *An exact sequence of metrized coherent sheaves with com-*

patible metrics is a commutative diagram

$$\begin{array}{ccccccccc} & & \vdots & & \vdots & & \vdots & & \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \to & \overline{E}_{n,1} & \to & \dots & \to & \overline{E}_{0,1} & \to & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \to & \overline{E}_{n,0} & \to & \dots & \to & \overline{E}_{0,0} & \to & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \to & \mathcal{F}_n & \to & \dots & \to & \mathcal{F}_0 & \to & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ & & 0 & & 0 & & 0 & & \end{array} \tag{2.23}$$

where all the rows and columns are exact. The columns of this diagram are the individual metrics of each coherent sheaf. We will say that an exact sequence with compatible metrics is *orthogonally split* if each row of vector bundles is an orthogonally split exact sequence of hermitian vector bundles.

As in the case of exact sequences of hermitian vector bundles, the Chern character form is not compatible with exact sequences of metrized coherent sheaves and we can define a secondary Bott-Chern character which measures the lack of compatibility between the metrics.

Theorem 2.24. *1) There is a unique way to attach to every finite exact sequence of metrized coherent sheaves with compatible metrics*

$$\overline{\varepsilon}\colon \qquad 0 \to \overline{\mathcal{F}}_n \to \cdots \to \overline{\mathcal{F}}_0 \to 0$$

on a complex manifold X a Bott-Chern secondary character

$$\widetilde{\mathrm{ch}}(\overline{\varepsilon}) \in \bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(X,p)$$

such that the following axioms are satisfied:

(i) (Differential equation)

$$\mathrm{d}_{\mathcal{D}}\, \widetilde{\mathrm{ch}}(\overline{\varepsilon}) = \sum_k (-1)^k \,\mathrm{ch}(\overline{\mathcal{F}_k}).$$

(ii) (Functoriality) If $f\colon X' \longrightarrow X$ is a morphism of complex manifolds, that is tor-independent from the coherent sheaves $\mathcal{F}_k$, then

$$f^*(\widetilde{\mathrm{ch}})(\overline{\varepsilon}) = \widetilde{\mathrm{ch}}(f^*\overline{\varepsilon}),$$

where the exact sequence $f^*\overline{\varepsilon}$ exists thanks to the tor-independence.

(iii) (Horizontal normalization) If $\overline{\varepsilon}$ is orthogonally split then

$$\widetilde{\mathrm{ch}}(\overline{\varepsilon}) = 0.$$

2) There is a unique way to attach to every finite exact sequence of metrized coherent sheaves

$$\overline{\varepsilon}\colon \qquad 0 \to \overline{\mathcal{F}}_n \to \dots \to \overline{\mathcal{F}}_0 \to 0$$

on a complex manifold X a Bott-Chern secondary character

$$\widetilde{\mathrm{ch}}(\overline{\varepsilon}) \in \bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(X,p)$$

such that the axioms (i), (ii) and (iii) above and the axiom (iv) below are satisfied:

(iv) (Vertical normalization) For every bounded complex of hermitian vector bundles

$$\dots \to \overline{A}_k \to \dots \to \overline{A}_0 \to 0$$

that is orthogonally split, and every bounded complex of metrized coherent sheaves

$$\overline{\varepsilon}\colon \qquad 0 \to \overline{\mathcal{F}}_n \to \dots \to \overline{\mathcal{F}}_0 \to 0$$

where the metrics are given by $\overline{E}_{i,*} \to \mathcal{F}_i$, if, for some i_0 we denote

$$\overline{\mathcal{F}}'_{i_0} = (\mathcal{F}_{i_0}, \overline{E}_{i_0,*} \oplus \overline{A}_* \to \mathcal{F}_{i_0})$$

and

$$\overline{\varepsilon}'\colon \qquad 0 \to \overline{\mathcal{F}}_n \to \dots \to \overline{\mathcal{F}}'_{i_0} \to \dots \to \overline{\mathcal{F}}_0 \to 0,$$

then $\widetilde{\mathrm{ch}}(\overline{\varepsilon}') = \widetilde{\mathrm{ch}}(\overline{\varepsilon})$.

Proof. 1) The uniqueness is proved using the standard deformation argument. By definition, the metrics of the coherent sheaves form a diagram like (2.23). On $X \times \mathbb{P}^1$, for each $j \geq 0$ we consider the exact sequences $\widetilde{E}_{*,j} = \mathrm{tr}_1(E_{*,j})$ associated to the rows of the diagram with the hermitian metrics of definition 2.9. Then, for each i,j there are maps $\mathrm{d}\colon \widetilde{E}_{i,j} \to \widetilde{E}_{i-1,j}$, and $\delta\colon \widetilde{E}_{i,j} \to \widetilde{E}_{i,j-1}$. We denote

$$\widetilde{\mathcal{F}}_i = \mathrm{Coker}(\delta\colon \widetilde{E}_{i,1} \to \widetilde{E}_{i,0}).$$

Using the definition of tr_1 and diagram chasing one can prove that there is a commutative diagram

$$\begin{array}{ccccccccc} & & \vdots & & \vdots & & \vdots & & \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \to & \widetilde{E}_{n,1} & \to & \dots & \to & \widetilde{E}_{0,1} & \to & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \to & \widetilde{E}_{n,0} & \to & \dots & \to & \widetilde{E}_{0,0} & \to & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \to & \widetilde{\mathcal{F}}_n & \to & \dots & \to & \widetilde{\mathcal{F}}_0 & \to & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ & & 0 & & 0 & & 0 & & \end{array} \tag{2.25}$$

where all the rows and columns are exact. In particular this implies that the inclusions $i_0\colon X \to X \times \{0\} \to X \times \mathbb{P}^1$ and $i_\infty\colon X \to X \times \{\infty\} \to X \times \mathbb{P}^1$ are tor-independent from the sheaves $\widetilde{\mathcal{F}}_i$. But $i_0^* \widetilde{\mathcal{F}}_*$ is isometric with $\overline{\mathcal{F}}_*$ and $i_\infty^* \widetilde{\mathcal{F}}_*$ is orthogonally split. Hence, by the standard argument, axioms (i), (ii) and (iii) imply that

$$\widetilde{\mathrm{ch}}(\overline{\varepsilon}) = \sum_j (-1)^j \widetilde{\mathrm{ch}}(\overline{E}_{*,j}). \tag{2.26}$$

To prove the existence we use equation (2.26) as definition. Then the properties of the Bott-Chern classes of exact sequences of hermitian vector bundles imply that axioms (i), (ii) and (iii) are satisfied.

Proof of 2). We first assume that such theory exists. Let

$$\dots \to \overline{A}_k \to \dots \to \overline{A}_0 \to 0$$

be a bounded complex of hermitian vector bundles, non necessarily orthogonally split, and

$$\overline{\varepsilon}\colon \qquad 0 \to \overline{\mathcal{F}}_n \to \dots \to \overline{\mathcal{F}}_0 \to 0$$

a bounded complex of metrized coherent sheaves where the metrics are given by $\overline{E}_{i,*} \to \mathcal{F}_i$. As in axiom (iv), for some i_0 we denote

$$\overline{\mathcal{F}}'_{i_0} = (\mathcal{F}_{i_0}, \overline{E}_{i,*} \oplus \overline{A}_* \to \mathcal{F}_{i_0})$$

and

$$\overline{\varepsilon}'\colon \qquad 0 \to \overline{\mathcal{F}}_n \to \dots \to \overline{\mathcal{F}}'_{i_0} \to \dots \to \overline{\mathcal{F}}_0 \to 0.$$

By axioms (i), (ii) and (iv), the class $(-1)^{i_0}(\widetilde{\mathrm{ch}}(\overline{\varepsilon}') - \widetilde{\mathrm{ch}}(\overline{\varepsilon}))$ satisfies the properties that characterize $\widetilde{\mathrm{ch}}(A_*)$. Therefore $\widetilde{\mathrm{ch}}(\overline{\varepsilon}') = \widetilde{\mathrm{ch}}(\overline{\varepsilon}) + (-1)^{i_0}\widetilde{\mathrm{ch}}(A_*)$.

Fix again a number i_0 and assume that there is an exact sequence of resolutions

$$\begin{array}{ccccccccc} 0 & \longrightarrow & \overline{A}_\bullet & \longrightarrow & \overline{E}'_{i_0,*} & \longrightarrow & \overline{E}_{i_0,*} & \longrightarrow & 0 \\ & & \downarrow & & \downarrow & & \downarrow & & \\ & & 0 & \longrightarrow & \mathcal{F}_{i_0} & = & \mathcal{F}_{i_0} & & \end{array} \tag{2.27}$$

Let now $\overline{\varepsilon}'$ denote the exact sequence $\overline{\varepsilon}$ but with the metric $\overline{E}'_{i_0,*}$ in the position i_0. Let $\overline{\eta}_j$ denote the j-th row of the diagram (2.27). Again using a deformation argument one sees that

$$\widetilde{\mathrm{ch}}(\overline{\varepsilon}') - \widetilde{\mathrm{ch}}(\overline{\varepsilon}) = (-1)^{i_0} \left(\widetilde{\mathrm{ch}}(\overline{A}_*) - \sum_j (-1)^j \, \widetilde{\mathrm{ch}}(\eta_j) \right). \tag{2.28}$$

Choose now a compatible system of metrics

$$\begin{array}{ccccccccc}
 & & \vdots & & \vdots & & \vdots & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \overline{D}_{n,1} & \to & \dots & \to & \overline{D}_{0,1} & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \overline{D}_{n,0} & \to & \dots & \to & \overline{D}_{0,0} & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \mathcal{F}_n & \to & \dots & \to & \mathcal{F}_0 & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & & 0 & & 0 & &
\end{array} \tag{2.29}$$

we denote by $\overline{\lambda}_j$ each row of the above diagram. For each i, choose a resolution $\overline{E}'_{i,*} \longrightarrow \mathcal{F}_i$ such that there exist exact sequences of resolutions

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \overline{A}_{i,*} & \longrightarrow & \overline{E}'_{i,*} & \longrightarrow & \overline{E}_{i,*} & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & \longrightarrow & \mathcal{F}_i & = & \mathcal{F}_i & &
\end{array} \tag{2.30}$$

and

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \overline{B}_{i,*} & \longrightarrow & \overline{E}'_{i,*} & \longrightarrow & \overline{D}_{i,*} & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & \longrightarrow & \mathcal{F}_i & = & \mathcal{F}_i & &
\end{array} \tag{2.31}$$

We denote by $\overline{\eta}_{i,j}$ each row of the diagram (2.30) and by $\overline{\mu}_{i,j}$ each row of the diagram (2.31). Then, by (2.28) and (2.26), we have

$$\begin{aligned}
\widetilde{\mathrm{ch}}(\overline{\varepsilon}) = \sum_j (-1)^j \, \widetilde{\mathrm{ch}}(\overline{\lambda}_j) + \sum_i (-1)^i (\widetilde{\mathrm{ch}}(\overline{B}_{i,*}) - \widetilde{\mathrm{ch}}(\overline{A}_{i,*})) \\
+ \sum_{i,j} (-1)^{i+j} (\widetilde{\mathrm{ch}}(\overline{\eta}_{i,j}) - \widetilde{\mathrm{ch}}(\overline{\mu}_{i,j}))
\end{aligned} \tag{2.32}$$

Thus, $\widetilde{\mathrm{ch}}(\overline{\varepsilon})$ is uniquely determined by axioms (i) to (iv). To prove the existence we use equation (2.32) as definition. We have to show that this definition is independent of the choices of the new resolutions. This independence follows from corollary 2.19. Once we know that the Bott-Chern classes are well defined, it is clear that they satisfy axioms (i), (ii), (iii) and (iv). □

Proposition 2.33. *(Compatibility with exact squares) If*

$$\begin{array}{ccccccccc} & & \vdots & & \vdots & & \vdots & & \\ & & \downarrow & & \downarrow & & \downarrow & & \\ \dots & \to & \overline{\mathcal{F}}_{n+1,m+1} & \to & \overline{\mathcal{F}}_{n+1,m} & \to & \overline{\mathcal{F}}_{n+1,m-1} & \to & \dots \\ & & \downarrow & & \downarrow & & \downarrow & & \\ \dots & \to & \overline{\mathcal{F}}_{n,m+1} & \to & \overline{\mathcal{F}}_{n,m} & \to & \overline{\mathcal{F}}_{n,m-1} & \to & \dots \\ & & \downarrow & & \downarrow & & \downarrow & & \\ \dots & \to & \overline{\mathcal{F}}_{n-1,m+1} & \to & \overline{\mathcal{F}}_{n-1,m} & \to & \overline{\mathcal{F}}_{n-1,m-1} & \to & \dots \\ & & \downarrow & & \downarrow & & \downarrow & & \\ & & \vdots & & \vdots & & \vdots & & \end{array}$$

is a bounded commutative diagram of metrized coherent sheaves, where all the rows $\dots(\overline{\varepsilon}_{n-1})$, $(\overline{\varepsilon}_n)$, $(\overline{\varepsilon}_{n+1})$, $\dots$ *and all the columns* $(\overline{\eta}_{m-1})$, $(\overline{\eta}_m)$, $(\overline{\eta}_{m+1})$ *are exact, then*

$$\sum_n (-1)^n \widetilde{\mathrm{ch}}(\overline{\varepsilon}_n) = \sum_m (-1)^m \widetilde{\mathrm{ch}}(\overline{\eta}_m).$$

Proof. This follows from equation (2.32) and corollary 2.19. □

We will use the notation of definition 2.13 also in the case of metrized coherent sheaves.
It is easy to verify the following result.

Proposition 2.34. *Let*

$$(\overline{\varepsilon}) \qquad \dots \longrightarrow \overline{E}_{n+1} \longrightarrow \overline{E}_n \longrightarrow \overline{E}_{n-1} \longrightarrow \dots$$

be a finite exact sequence of hermitian vector bundles. Then the Bott-Chern classes obtained by theorem 2.24 and by theorem 2.3 agree. □

Proposition 2.35. *Let* $\overline{\mathcal{F}} = (\mathcal{F}, \overline{E}_* \to \mathcal{F})$ *be a metrized coherent sheaf. We consider the exact sequence of metrized coherent sheaves*

$$\overline{\varepsilon}\colon \qquad 0 \longrightarrow \overline{E}_n \to \dots \to \overline{E}_0 \to \overline{\mathcal{F}} \to 0,$$

where, by abuse of notation, $\overline{E}_i = (E_i, \overline{E}_i \overset{=}{\to} E_i)$. *Then* $\widetilde{\mathrm{ch}}(\overline{\varepsilon}) = 0$.

Proof. Define $\mathcal{K}_i = \mathrm{Ker}(E_i \to E_{i-1})$, $i = 1, \dots, n$ and $\mathcal{K}_0 = \mathrm{Ker}(E_0 \to \mathcal{F})$. Write

$$\overline{\mathcal{K}_i} = (\mathcal{K}_i, 0 \to \overline{E}_n \to \dots \to \overline{E}_{i+1} \to \mathcal{K}_i),\ i = 0, \dots, n,$$

and $\overline{\mathcal{K}}_{-1} = \overline{\mathcal{F}}$. If we prove that

$$\widetilde{\mathrm{ch}}(0 \to \overline{\mathcal{K}_i} \to \overline{E}_i \to \overline{\mathcal{K}}_{i-1} \to 0) = 0, \tag{2.36}$$

then we obtain the result by induction using proposition 2.33. In order to prove equation (2.36) we apply equation (2.32). To this end consider resolutions

$$\begin{aligned} \overline{D}_{0,*} &\longrightarrow \mathcal{K}_{i-1}, & \overline{D}_{0,k} &= \overline{E}_{k+i} \\ \overline{D}_{1,*} &\longrightarrow E_{i}, & \overline{D}_{1,k} &= \overline{E}_{k+i+1} \oplus \overline{E}_{k+i} \\ \overline{D}_{2,*} &\longrightarrow \mathcal{K}_{i}, & \overline{D}_{2,k} &= \overline{E}_{k+i+1} \end{aligned}$$

with the map $D_{2,k} \overset{\Delta}{\to} D_{1,k}$ given by $s \mapsto (s, \mathrm{d}\, s)$ and the map $D_{1,k} \overset{\nabla}{\to} D_{0,k}$ given by $(s,t) \mapsto t - \mathrm{d}\, s$. The differential of the complex $D_{1,k}$ is given by $(s,t) \mapsto (t,0)$. Using equations (2.32) and (2.26) we write the left hand side of equation (2.36) in terms of Bott-Chern classes of vector bundles. All the exact sequences involved are orthogonally split except maybe the sequences

$$\overline{\lambda}_k\colon \qquad 0 \to \overline{D}_{2,k} \to \overline{D}_{1,k} \to \overline{D}_{0,k} \to 0.$$

But now we consider the diagrams

$$\begin{array}{ccccc} \overline{E}_{k+i+1} & \xrightarrow{i_1} & \overline{E}_{k+i+1} \oplus \overline{E}_{k+i} & \xrightarrow{p_2} & \overline{E}_{k+i} \\ \Big\downarrow \mathrm{id} & & \Big\downarrow f & & \Big\downarrow \mathrm{id} \\ \overline{E}_{k+i+1} & \xrightarrow{\Delta} & \overline{E}_{k+i+1} \oplus \overline{E}_{k+i} & \xrightarrow{\nabla} & \overline{E}_{k+i} \end{array}$$

and

$$\begin{array}{ccccc} \overline{E}_{k+i} & \xrightarrow{i_2} & \overline{E}_{k+i+1} \oplus \overline{E}_{k+i} & \xrightarrow{p_1} & \overline{E}_{k+i+1}\ , \\ \Big\downarrow \mathrm{id} & & \Big\downarrow f & & \Big\downarrow \mathrm{id} \\ \overline{E}_{k+i} & \xrightarrow{i_2} & \overline{E}_{k+i+1} \oplus \overline{E}_{k+i} & \xrightarrow{p_1} & \overline{E}_{k+i+1} \end{array}$$

where i_i, i_2 are the natural inclusions, p_1 and p_2 are the projections and $f(s,t) = (s, t + f(s))$. These diagrams and corollary 2.19 imply that $\widetilde{\mathrm{ch}}(\overline{\lambda}_k) = 0$. □

Remark 2.37. In [32], Zha shows that the Bott-Chern classes associated to exact sequences of metrized coherent sheaves are characterized by proposition 2.34, proposition 2.35 and proposition 2.33. We prefer the characterization in terms of the differential equation, the functoriality and the normalization, because it relies on natural extensions of the corresponding axioms that define the Bott-Chern classes for exact sequences of hermitian vector bundles. Moreover, this approach will be used in a subsequent paper where we will study singular Bott-Chern classes associated to arbitrary proper morphisms.

The following generalization of proposition 2.35 will be useful later. Let

$$\varepsilon\colon 0 \to \mathcal{G}_n \to \mathcal{G}_{n-1} \to \cdots \to \mathcal{G}_0 \to \mathcal{F} \to 0$$

be a finite resolution of a coherent sheaf by coherent sheaves. Assume that we have a commutative diagram

$$\begin{array}{ccccccccccc}
 & & \vdots & & \vdots & & \vdots & & & & \\
 & & \downarrow & & \downarrow & & \downarrow & & & & \\
 & & \overline{E}_{1,n} & \to & \dots & \to & \overline{E}_{1,0} & & & & \\
 & & \downarrow & & \downarrow & & \downarrow & & & & \\
 & & \overline{E}_{0,n} & \to & \dots & \to & \overline{E}_{0,0} & & & & \\
 & & \downarrow & & \downarrow & & \downarrow & & & & \\
0 & \to & \overline{\mathcal{G}}_n & \to & \dots & \to & \overline{\mathcal{G}}_0 & \to & \mathcal{F} & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & & & \\
 & & 0 & & 0 & & 0 & & & &
\end{array}$$

where the columns are exact, the rows are complexes and the $\overline{E}_{i,j}$ are hermitian vector bundles. The columns of this diagram define metrized coherent sheaves $\overline{\mathcal{G}}_i$. Let $\overline{\mathcal{F}}$ be the metrized coherent sheaf defined by the resolution $\mathrm{Tot}(\overline{E}_{*,*}) \longrightarrow \mathcal{F}$.

Proposition 2.38. *With the notations above, let $\overline{\varepsilon}$ be the exact sequence of metrized coherent sheaves*

$$\overline{\varepsilon}\colon 0 \to \overline{\mathcal{G}}_n \to \overline{\mathcal{G}}_{n-1} \to \cdots \to \overline{\mathcal{G}}_0 \to \overline{\mathcal{F}} \to 0$$

Then $\widetilde{\mathrm{ch}}(\overline{\varepsilon}) = 0$.

Proof. For each k, let $\mathrm{Tot}_k = \mathrm{Tot}((E_{*,j})_{j\geq k})$. There are inclusions $\mathrm{Tot}_k \longrightarrow \mathrm{Tot}_{k-1}$. Let $\overline{D}_{*,j} = s(\mathrm{Tot}_{j+1} \to \mathrm{Tot}_j)$ with the hermitian metric induced by $\overline{E}_{*,*}$. There are exact sequences of complexes

$$0 \longrightarrow \overline{E}_{*,j} \longrightarrow \overline{D}_{*,j} \longrightarrow s(\mathrm{Tot}_{j+1} \to \mathrm{Tot}_{j+1}) \longrightarrow 0 \qquad (2.39)$$

that are orthogonally split at each degree. The third complex is orthogonally split. Therefore, if we denote by h_E and h_D the metric structures of $\mathcal{G}_j$ induced respectively by the first and second column of diagram (2.39), then

$$\widetilde{\mathrm{ch}}(\mathcal{G}_j, h_E, h_D) = 0. \qquad (2.40)$$

There is a commutative diagram of resolutions

$$\begin{array}{ccccccccccccc}
 & & \vdots & & \vdots & & \vdots & & \vdots & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \overline{D}_{1,n} & \to & \dots & \to & \overline{D}_{1,0} & \to & (\mathrm{Tot}_0)_1 & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \overline{D}_{0,n} & \to & \dots & \to & \overline{D}_{0,0} & \to & (\mathrm{Tot}_0)_0 & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \mathcal{G}_n & \to & \dots & \to & \mathcal{G}_0 & \to & \mathcal{F} & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & & 0 & & 0 & & 0 & &
\end{array}$$

where the rows of degree greater or equal than zero are orthogonally split. Hence the result follows from equation (2.26), equation (2.40) and proposition 2.33. □

Remark 2.41. We have only defined the Bott-Chern classes associated to the Chern character. Everything applies without change to any additive characteristic class. The reader will find no difficulty to adapt the previous results to any multiplicative characteristic class like the Todd genus or the total Chern class.

3 Direct images of Bott-Chern classes

The aim of this section is to show that certain direct images of Bott-Chern classes are closed. This result is a generalization of results of Bismut, Gillet and Soulé [6] page 325 and of Mourougane [29] proposition 6. The fact that these direct images of Bott-Chern classes are closed implies that certain relations between characteristic classes are true at the level of differential forms (see corollary 3.7 and corollary 3.8).

In the first part of this section we deal with differential geometry. Thus all the varieties will be differentiable manifolds.

Let G_1 be a Lie group and let $\pi\colon N_2 \longrightarrow M_2$ be a principal bundle with structure group G_2 and connection ω_2. Assume that there is a left action of G_1 over N_2 that commutes with the right action of G_2 and such that the connection ω_2 is G_1-invariant.

Let $\mathfrak{g}_1$ and $\mathfrak{g}_2$ be the Lie algebras of G_1 and G_2. Every element $\gamma \in \mathfrak{g}_1$ defines a tangent vector field γ^* over N_2 given by

$$\gamma^*_p = \left.\frac{d}{dt}\right|_{t=0} \exp(t\gamma)p.$$

Let $(\gamma^*)^V$ be the vertical component of γ^* with respect to the connection ω_2. For every point $p \in N_2$, we denote by $\varphi(\gamma, p) \in \mathfrak{g}_2$ the element characterized by $(\gamma^*)^V_p = \varphi(\gamma, p)^*_p$, where $\varphi(\gamma, p)^*$ is the fundamental vector field associated to $\varphi(\gamma, p)$.

The commutativity of the actions of G_1 and G_2 and the invariance of the connection ω_2 implies that, for $g \in G_1$ and $\gamma \in \mathfrak{g}_1$, the following equalities hold

$$L_{g*}(\gamma^*) = (\operatorname{ad}(g)\gamma^*), \tag{3.1}$$

$$L_{g*}(\gamma^*)^V = (\operatorname{ad}(g)\gamma^*)^V, \tag{3.2}$$

$$\varphi(\operatorname{ad}(g)\gamma, p) = \varphi(\gamma, g^{-1}p). \tag{3.3}$$

Let $\mathcal{G}_2$ be the vector bundle over M_2 associated to N_2 and the adjoint representation of G_2. That is,

$$\mathcal{G}_2 = N_2 \times \mathfrak{g}_2 \,/\big\langle (pg, v) \sim (p, \operatorname{ad}(g)v)\big\rangle \,.$$

Thus, we can identify smooth sections of $\mathcal{G}_2$ with $\mathfrak{g}_2$-valued functions on N_2 that are invariant under the action of G_2. In this way, $\varphi(\gamma, p)$ determines a section

$$\varphi(\gamma) \in C^\infty(N_2, \mathfrak{g}_2)^{G_2} = C^\infty(M_2, \mathcal{G}_2).$$

Equation (3.3) implies that, for $g \in G_1$ and $\gamma \in \mathfrak{g}_1$,

$$\varphi(\mathrm{ad}(g)\gamma) = L^*_{g^{-1}}\varphi(\gamma).$$

We denote by Ω^{ω_2} the curvature of the connection ω_2. Let P be an invariant function on $\mathfrak{g}_2$, then $P(\Omega^{\omega_2} + \varphi(\gamma))$ is a well defined differential form on M_2.

Proposition 3.4. *Let P be an invariant function on $\mathfrak{g}_2$ and let μ be a current on M_2 invariant under the action of G_1. Then $\mu(P(\Omega^{\omega_2}+\varphi(\gamma)))$ is an invariant function on $\mathfrak{g}_1$.*

Proof. Let $g \in G_1$. Then,

$$\begin{aligned}
\mu(P(\Omega^{\omega_2} + \varphi(\mathrm{ad}(g)\gamma))) &= \mu(P(\Omega^{\omega_2} + L^*_{g^{-1}}\varphi(\gamma))) \\
&= \mu(P(L^*_{g^{-1}}\Omega^{\omega_2} + L^*_{g^{-1}}\varphi(\gamma))) \\
&= L_{g^{-1}*}(\mu)(P(\Omega^{\omega_2} + \varphi(\gamma))) \\
&= \mu(P(\Omega^{\omega_2} + \varphi(\gamma)))
\end{aligned}$$

□

Let now $N_1 \longrightarrow M_1$ be a principal bundle with structure group G_1 and provided with a connection ω_1. Then we can form the diagram

$$\begin{array}{ccc}
N_1 \times N_2 & \xrightarrow{\pi_1} & N_1 \underset{G_1}{\times} N_2 \\
\Big\downarrow \pi' & & \Big\downarrow \pi \\
N_1 \times M_2 & \xrightarrow{\pi_2} & N_1 \underset{G_1}{\times} M_2 \\
& & \Big\downarrow q \\
& & M_1
\end{array}$$

Then π is a principal bundle with structure group G_2. The connections ω_1 and ω_2 induce a connection on the principal bundle π. The subbundle of horizontal vectors with respect to this connection is given by $\pi_{1*}(T^H N_1 \oplus T^H N_2)$. We will denote this connection by $\omega_{1,2}$. We are interested in computing the curvature $\omega_{1,2}$.

In fact, all the maps in the above diagram are fiber bundles provided with a connection. When applicable, given a vector field U in any of these spaces, we will denote by $U^{H,1}$ the horizontal lifting to $N_1 \times N_2$, by $U^{H,2}$ the horizontal lifting to $N_1 \underset{G_1}{\times} N_2$ and by $U^{H,3}$ the horizontal lifting to $N_1 \underset{G_1}{\times} M_2$.

The tangent space $T(N_1 \times N_2)$ can be decomposed as direct sum in the following ways

$$\begin{aligned} T(N_1 \times N_2) &= T^H N_1 \oplus T^V N_1 \oplus T^H N_2 \oplus T^V N_2 \\ &= T^H N_1 \oplus T^V N_1 \oplus T^H N_2 \oplus \operatorname{Ker} \pi_{1*}, \end{aligned} \tag{3.5}$$

For every point $(x, y) \in N_1 \times N_2$ we have that $(\operatorname{Ker} \pi_{1*})_{(x,y)} \subset T^V_x N_1 \oplus T_y N_2$. Moreover, there is an isomorphism $\mathfrak{g}_1 \longrightarrow (\operatorname{Ker} \pi_{1*})_{(x,y)}$ that sends an element $\gamma \in \mathfrak{g}_1$ to the element $(\gamma^*_x, -\gamma^*_y) \in T^V_x N_1 \oplus T_y N_2$.
The tangent space to $N_1 \underset{G_1}{\times} M_2$ can be decomposed as the sum of the subbundle of vertical vectors with respect to q and the subbundle of horizontal vectors defined by the connection ω_1. The horizontal lifting to $N_1 \times N_2$ of a vertical vector lies in $T^H N_2$ and the horizontal lifting of a horizontal vector lies in $T^H N_1$.
Let U, V be two vector fields on M_1 and let $U^{H,3}$, $V^{H,3}$ be the horizontal liftings to $N_1 \underset{G_1}{\times} M_2$. Then

$$\begin{aligned} \Omega^{\omega_{1,2}}(U^{H,3}, V^{H,3}) &= [U^{H,3}, V^{H,3}]^{H,2} - [U^{H,2}, V^{H,2}] \\ &= \pi_{1*}([U^{H,3}, V^{H,3}]^{H,1} - [U^{H,1}, V^{H,1}]) \\ &= \pi_{1*}([U^{H,3}, V^{H,3}]^{H,1} - [U, V]^{H,1} + [U, V]^{H,1} - [U^{H,1}, V^{H,1}]) \\ &= \pi_{1,*}([U^{H,3}, V^{H,3}]^{H,1} - [U, V]^{H,1} + \Omega^{\omega_1}(U, V)). \end{aligned}$$

But, we have

$$\begin{aligned} \Omega^{\omega_{1,2}}(U^{H,3}, V^{H,3}) &\in T^V N_2, \\ \Omega^{\omega_1}(U, V) &\in T^V N_1, \\ [U^{H,3}, V^{H,3}]^{H,1} - [U, V]^{H,1} &\in T^H N_2. \end{aligned}$$

Therefore, by the direct sum decomposition (3.5) we obtain that

$$\Omega^{\omega_{1,2}}(U^{H,3}, V^{H,3}) = ((\pi_{1*} \Omega^{\omega_1}(U, V)))^V,$$

where the vertical part is taken with respect to the fib re bundle π.
If U is a horizontal vector field over $N_1 \underset{G_1}{\times} M_2$ and V is a vertical vector field, a similar argument shows that $\Omega^{\omega_{1,2}}(U, V) = 0$. Finally, if U and V are vector fields on M_2, they determine vertical vector fields on $N_1 \underset{G_1}{\times} M_2$. Then the horizontal liftings $U^{H,1}$ and $V^{H,1}$ are induced by horizontal liftings of U and V to N_2. Therefore, reasoning as before we see that

$$\Omega^{\omega_{1,2}}(U, V) = \Omega^{\omega_2}(U, V).$$

Proposition 3.6. *Let G_1 and G_2 be Lie groups, with Lie algebras $\mathfrak{g}_1$ and $\mathfrak{g}_2$. For $i = 1, 2$, let $N_i \longrightarrow M_i$ be a principal bundle with structure group*

G_i, provided with a connection ω_i. Assume that there is a left action of G_1 over N_2 that commutes with the right action of G_2 and that the connection ω_2 is invariant under the G_1-action. We form the G_2-principal bundle $\pi\colon N_1 \underset{G_1}{\times} N_2 \longrightarrow N_1 \underset{G_1}{\times} M_2$ with the induced connection $\omega_{1,2}$ and curvature $\Omega^{\omega_{1,2}}$. Let P be any invariant function on $\mathfrak{g}_2$. Thus $P(\Omega^{\omega_{1,2}})$ is a well defined closed differential form on $N_1 \underset{G_1}{\times} M_2$. Let μ be a current on M_2 invariant under the G_1-action. Being G_1 invariant, the current μ induces a current on $N_1 \underset{G_1}{\times} M_2$, that we denote also by μ. Let $q\colon N_1 \underset{G_1}{\times} M_2 \longrightarrow M_1$ be the projection. Then $q_*(P(\Omega^{\omega_{1,2}}) \wedge \mu)$ is a closed differential form on M_1.

Proof. Let $U \subset M_1$ be a trivializing open subset for N_1 and choose a trivialization of $N_1 |_U \cong U \times G_1$. With this trivialization, we can identify $\Omega^{\omega_1} |_U$ with a 2-form on U with values in $\mathfrak{g}_1$.
For $\gamma \in \mathfrak{g}_1$, we denote by

$$\psi_\mu(\gamma) = \mu(P(\Omega^{\omega_2} + \varphi(\gamma)))$$

the invariant function provided by proposition 3.4.
Then

$$q_*(P(\Omega^{\omega_{1,2}}) \wedge \mu) = \psi_\mu(\Omega^{\omega_1}).$$

Therefore, the result follows from the usual Chern-Weil theory. □

We go back now to complex geometry and analytic real Deligne cohomology and to the notations 1.3, in particular (1.4).

Corollary 3.7. *Let X be a complex manifold and let $\overline{E} = (E, h^E)$ be a rank r hermitian holomorphic vector bundle on X. Let $\pi\colon \mathbb{P}(E) \longrightarrow X$ be the associated projective bundle. On $\mathbb{P}(E)$ we consider the tautological exact sequence*

$$\overline{\xi}\colon 0 \longrightarrow \overline{\mathcal{O}(-1)} \longrightarrow \pi^*\overline{E} \longrightarrow \overline{Q} \longrightarrow 0$$

where all the vector bundles have the induced metric. Let P_1, P_2 and P_3 be invariant power series in 1, $r-1$ and r variables respectively with coefficients in $\mathbb{D}$. Let $P_1(\overline{\mathcal{O}(-1)})$ and $P_2(\overline{Q})$ be the associated Chern forms and let $\widetilde{P}_3(\overline{\xi})$ the associated Bott-Chern class. Then

$$\pi_*(P_1(\overline{\mathcal{O}(-1)}) \bullet P_2(\overline{Q}) \bullet \widetilde{P}_3(\overline{\xi})) \in \bigoplus_k \widetilde{\mathcal{D}}^{2k-1}(X,k)$$

is closed. Hence it defines a class in analytic real Deligne cohomology. This class does not depend on the hermitian metric of E.

Proof. We consider $\mathbb{C}^r$ with the standard hermitian metric. On the space $\mathbb{P}(\mathbb{C}^r)$ we have the tautological exact sequence

$$0 \longrightarrow \mathcal{O}_{\mathbb{P}(\mathbb{C}^r)}(-1) \xrightarrow{f} \mathbb{C}^r \longrightarrow Q \longrightarrow 0.$$

Let $(x:y)$ be homogeneous coordinates on $\mathbb{P}^1$ and let $t=x/y$ be the absolute coordinate. Let p_1 and p_2 be the two projections of $M_2=\mathbb{P}(\mathbb{C}^r)\times\mathbb{P}^1$. Let $\widetilde{E}$ be the cokernel of the map

$$\begin{array}{ccc} p_1^*\mathcal{O}_{\mathbb{P}(\mathbb{C}^r)}(-1) & \longrightarrow & p_1^*\mathcal{O}_{\mathbb{P}(\mathbb{C}^r)}(-1)\otimes p_2^*\mathcal{O}_{\mathbb{P}^1}(1)\oplus p_1^*\mathbb{C}^r\otimes p_2^*\mathcal{O}_{\mathbb{P}^1}(1)\\ s & \longmapsto & s\otimes y+f(s)\otimes x \end{array}$$

with the metric induced by the standard metric of $\mathbb{C}^r$ and the Fubini-Study metric of $\mathcal{O}_{\mathbb{P}(1)}(1)$.

Let N_2 be the principal bundle over M_2 formed by the triples (e_1,e_2,e_3), where e_1, e_2 and e_3 are unitary frames of $p_1^*\mathcal{O}_{\mathbb{P}(\mathbb{C}^r)}(-1)$, p_1^*Q and $\widetilde{E}$ respectively. The structure group of this principal bundle is $G_2=U(1)\times U(r-1)\times U(r)$. Let ω_2 be the connection induced by the hermitian holomorphic connections on the vector bundles $p_1^*\mathcal{O}_{\mathbb{P}(\mathbb{C}^r)}(-1)$, p_1^*Q and $\widetilde{E}$.

Now we denote $M_1=X$, and let N_1 be the bundle of unitary frames of $\overline{E}$. This is a principal bundle over M_1 with structure group $G_1=U(r)$.

The group G_1 acts on the left on N_2. This action commutes with the right action of G_2 and the connection ω_2 is invariant under this action.

Let $\mu=[-\log(|t|)]$ be the current on M_2 associated to the locally integrable function $-\log(|t|)$. This current is invariant under the action of G_1 because this group acts trivially on the factor $\mathbb{P}^1$.

The invariant power series P_1, P_2 and P_3 determine an invariant function P on $\mathfrak{g}_2$, the Lie algebra of G_2.

Let ω_1 be the connection induced in N_1 by the holomorphic hermitian connection on $\overline{E}$. As before let $\omega_{1,2}$ be the connection on $N_1\underset{G_1}{\times}N_2$ induced by ω_1 and ω_2 and let $q\colon N_1\underset{G_1}{\times}M_2\longrightarrow M_1$ be the projection. Observe that $N_1\underset{G_1}{\times}M_2=\mathbb{P}(E)\times\mathbb{P}^1$ and $q=\pi\circ p_1$.

By the projection formula and the definition of Bott-Chern classes we have

$$\pi_*(P_1(\overline{\mathcal{O}(-1)})\wedge P_2(\overline{Q})\wedge\widetilde{P}_3(\overline{\xi}))=q_*(\mu\bullet P(\Omega^{\omega_{1,2}})),$$

Therefore the fact that it is closed follows from 3.6. Since, for fixed P_1, P_2 and P_3, the construction is functorial on $(X.\overline{E})$, the fact that the class in analytic real Deligne cohomology does not depend on the choice of the hermitian metric follows from proposition 1.7. □

Corollary 3.8. *Let $\overline{E}=(E,h^E)$ be a hermitian holomorphic vector bundle on a complex manifold X. We consider the projective bundle $\pi\colon\mathbb{P}(E\oplus\mathbb{C})\longrightarrow X$. Let $\overline{Q}$ be the universal quotient bundle on the space $\mathbb{P}(E\oplus\mathbb{C})$ with the induced metric. Then the following equality of differential forms holds*

$$\pi_*\sum_i(-1)^i\operatorname{ch}(\bigwedge^i\overline{Q}^\vee)=\pi_*(c_r(\overline{Q})\operatorname{Td}^{-1}(\overline{Q}))=\operatorname{Td}^{-1}(\overline{E}).$$

Proof. Let $\overline{\xi}$ be the tautological exact sequence with induced metrics. We first prove that

$$\pi_*(c_r(\overline{Q})\,\mathrm{Td}(\overline{\mathcal{O}(-1)})) = 1.$$

We can write $\mathrm{Td}(\overline{\mathcal{O}(-1)}) = 1 + c_1(\overline{\mathcal{O}(-1)})\phi(\overline{\mathcal{O}(-1)})$ for certain power series ϕ. Since $c_{r+1}(\overline{E}\oplus\mathbb{C}) = 0$ we have

$$c_r(\overline{Q})c_1(\overline{\mathcal{O}(-1)}) = \mathrm{d}_{\mathcal{D}}\,\widetilde{c}_{r+1}(\overline{\xi}).$$

Therefore, by corollary 3.7, we have

$$\begin{aligned}\pi_*(c_r(\overline{Q})\,\mathrm{Td}(\overline{\mathcal{O}(-1)})) &= \pi_*(c_r(\overline{Q})) + \pi_*(c_r(\overline{Q})c_1(\overline{\mathcal{O}(-1)})\phi(\overline{\mathcal{O}(-1)}))\\ &= 1 + \mathrm{d}_{\mathcal{D}}\,\pi_*(\widetilde{c}_{r+1}(\overline{\xi})\phi(\overline{\mathcal{O}(-1)}))\\ &= 1.\end{aligned}$$

Then the corollary follows from corollary 3.7 by using the identity

$$\begin{aligned}\pi_*(c_r(\overline{Q})\,\mathrm{Td}^{-1}(\overline{Q})) = \pi_*(c_r(\overline{Q})\,\mathrm{Td}(\overline{\mathcal{O}(-1)})\pi^*\,\mathrm{Td}^{-1}(\overline{E}))\\ + \mathrm{d}_{\mathcal{D}}\,\pi_*(c_r(\overline{Q})\,\mathrm{Td}(\overline{\mathcal{O}(-1)})\widetilde{\mathrm{Td}^{-1}}(\overline{\xi})).\end{aligned}$$

□

The following generalization of corollary 3.7 provides many relations between integrals of Bott-Chern classes and is left to the reader.

Corollary 3.9. *Let X be a complex manifold and let $\overline{E} = (E, h^E)$ be a rank r hermitian holomorphic vector bundle on X. Let $\pi\colon \mathbb{P}(E) \longrightarrow X$ be the associated projective bundle. On $\mathbb{P}(E)$ we consider the tautological exact sequence*

$$\overline{\xi}\colon 0 \longrightarrow \overline{\mathcal{O}(-1)} \longrightarrow \pi^*\overline{E} \longrightarrow \overline{Q} \longrightarrow 0$$

where all the vector bundles have the induced metric. Let P_1 and P_2 be invariant power series in 1 and $r-1$ variables respectively with coefficients in $\mathbb{D}$ and let $P_3, \dots, P_k$ be invariant power series in r variables with coefficients in $\mathbb{D}$. Let $P_1(\overline{\mathcal{O}(-1)})$ and $P_2(\overline{Q})$ be the associated Chern forms and let $\widetilde{P}_3(\overline{\xi}), \dots, \widetilde{P}_k(\overline{\xi})$ be the associated Bott-Chern classes. Then

$$\pi_*(P_1(\overline{\mathcal{O}(-1)}) \bullet P_2(\overline{Q}) \bullet \widetilde{P}_3(\overline{\xi}) \bullet \cdots \bullet \widetilde{P}_k(\overline{\xi}))$$

is a closed differential form on X for any choice of the ordering in computing the non associative product under the integral.

4 Cohomology of currents and wave front sets

The aim of this section is to prove the Poincaré lemma for the complex of currents with fixed wave front set. This implies in particular a certain $\partial\bar{\partial}$-lemma (corollary 4.7) that will allow us to control the singularities of singular Bott-Chern classes.

Let X be a complex manifold of dimension n. Following notation 1.3 recall that there is a canonical isomorphism

$$H^*_{\mathcal{D}^{\mathrm{an}}}(X,\mathbb{R}(p)) \cong H^*(\mathcal{D}^*_D(X,p)).$$

A current η can be viewed as a generalized section of a vector bundle and, as such, has a wave front set that is denoted by $\mathrm{WF}(\eta)$. The theory of wave front sets of distributions is developed in [25] chap. VIII. For the theory of wave front sets of generalized sections, the reader can consult [24] chap. VI. Although we will work with currents and hence with generalized sections of vector bundles, we will follow [25].

The wave front set of η is a closed conical subset of the cotangent bundle of X minus the zero section $T^*X_0 = T^*X \setminus \{0\}$. This set describes the points and directions of the singularities of η and it allows us to define certain products and inverse images of currents.

Let $S \subset T^*X_0$ be a closed conical subset, we will denote by $\mathscr{D}^*_{X,S}$ the subsheaf of currents whose wave front set is contained in S. We will denote by $D^*(X,S)$ its complex of global sections.

For every open set $U \subset X$ there is an appropriate notion of convergence in $\mathscr{D}^*_{X,S}(U)$ (see [25] VIII Definition 8.2.2). All references to continuity below are with respect to this notion of convergence.

We next summarize the basic properties of wave front sets.

Proposition 4.1. *Let u be a generalized section of a vector bundle and let P be a differential operator with smooth coefficients. Then*

$$\mathrm{WF}(Pu) \subseteq \mathrm{WF}(u).$$

Proof. This is [25] VIII (8.1.11). □

Corollary 4.2. *The sheaf $\mathscr{D}^*_{X,S}$ is closed under ∂ and $\bar{\partial}$. Therefore it is a sheaf of Dolbeault complexes.*

Let $f\colon X \longrightarrow Y$ be a morphism of complex manifolds. The *set of normal directions* of f is

$$N_f = \{(f(x),v) \in T^*Y \mid df(x)^t v = 0\}.$$

This set measures the singularities of f. For instance, if f is a smooth map then $N_f = 0$ whereas, if f is a closed immersion, N_f is the conormal bundle of $f(X)$. Let $S \subset T^*Y_0$ be a closed conical subset. We will say that f is transverse to S if $N_f \cap S = \emptyset$. We will denote

$$f^*S = \{(x, df(x)^t v) \in T^*X_0 \mid (f(x),v) \in S\}.$$

Theorem 4.3. *Let $f\colon X \longrightarrow Y$ be a morphism of complex manifolds that is transverse to S. Then there exists one and only one extension of the pull-back morphism $f^*\colon \mathscr{E}^*_Y \longrightarrow \mathscr{E}^*_X$ to a continuous morphism*

$$f^*\colon \mathscr{D}^*_{Y,S} \longrightarrow \mathscr{D}^*_{X,f^*S}.$$

In particular there is a continuous morphism of complexes

$$D^*(Y,S) \longrightarrow D^*(X,f^*S).$$

Proof. This follows from [25] theorem 8.2.4. □

We now recall the effect of correspondences on the wave front sets.
Let $K \in D^*(X \times Y)$, and let S be a conical subset of T^*Y_0. We will write

$$\begin{aligned} \mathrm{WF}(K)_X &= \{(x,\xi) \in T^*X_0 \mid \exists y \in Y, (x,y,\xi,0) \in \mathrm{WF}(K)\} \\ \mathrm{WF}'(K)_Y &= \{(y,\eta) \in T^*Y_0 \mid \exists x \in X, (x,y,0,-\eta) \in \mathrm{WF}(K)\} \\ \mathrm{WF}'(K) \circ S &= \{(x,\xi) \in T^*X_0 \mid \exists (y,\eta) \in S, (x,y,\xi,-\eta) \in \mathrm{WF}(K)\}. \end{aligned}$$

Theorem 4.4. *The image of the correspondence map*

$$\begin{array}{ccc} E^*_c(Y) & \longrightarrow & D^*(X) \\ \eta & \longmapsto & p_{1*}(K \wedge p_2^*(\eta)) \end{array}$$

is contained in $D^*(X, WF(K)_X)$*. Moreover, if* $S \cap \mathrm{WF}'(K)_Y = \emptyset$*, then there exists one and only one extension to a continuous map*

$$D^*_c(Y,S) \longrightarrow D^*(X,S'),$$

where $S' = \mathrm{WF}(K)_X \cup \mathrm{WF}'(K) \circ S$.

Proof. This is [25] theorem 8.2.13. □

We are now in a position to state and prove the Poincaré lemma for currents with fixed wave front set. As usual, we will denote by F the Hodge filtration of any Dolbeault complex.

Theorem 4.5 (Poincaré lemma). *Let S be any conical subset of T^*X_0. Then the natural morphism*

$$\iota\colon (E^*(X),F) \longrightarrow (D^*(X,S),F)$$

is a filtered quasi-isomorphism.

Proof. Let K be the Bochner-Martinelli integral operator on $\mathbb{C}^n \times \mathbb{C}^n$. It is the operator

$$\begin{array}{ccc} E^{p,q}_c(\mathbb{C}^n) & \longrightarrow & E^{p,q-1}(\mathbb{C}^n) \\ \varphi & \longmapsto & \int_{w\in\mathbb{C}^n} k(z,w)\wedge\varphi(w), \end{array}$$

where k is the Bochner-Martinelli kernel ([21] pag. 383). Thus k is a differential form on $\mathbb{C}^n \times \mathbb{C}^n$ with singularities only along the diagonal.
Using the explicit description of k in [21], it can be seen that $WF(k) = N^*\Delta_0$, the conormal bundle of the diagonal. By theorem 4.4, the operator K defines a continuous linear map from $\Gamma_c(\mathbb{C}^n, \mathscr{D}^*_{\mathbb{C}^n,S})$ to $\Gamma(\mathbb{C}^n, \mathscr{D}^*_{\mathbb{C}^n,S})$. This is the key

fact that allows us to adapt the proof of the Poincaré Lemma for arbitrary currents to the case of currents with fixed wave front set.
We will prove that the sheaf inclusion

$$(\mathscr{E}_X, F) \longrightarrow (\mathscr{D}_{X,S}, F)$$

is a filtered quasi-isomorphism. Then the theorem will follow from the fact that both are fine sheaves.
The previous statement is equivalent to the fact that, for any integer $p \geq 0$, the inclusion

$$\iota\colon \mathscr{E}_X^{p,*} \longrightarrow \mathscr{D}_{X,S}^{p,*}$$

is a quasi-isomorphism.
Let $x \in X$, since exactness can be checked at the level of stalks, we need to show that

$$\iota_x\colon \mathscr{E}_{X,x}^{p,*} \longrightarrow \mathscr{D}_{X,S,x}^{p,*}$$

is a quasi-isomorphism. let U be a coordinate neighborhood around x and let $x \in V \subset U$ be a relatively compact open subset.
Let $\rho \in C_c^\infty(U)$ be a function with compact support such that $\rho\mid_V = 1$. We define an operator

$$K\rho\colon \mathscr{D}_{X,S}^{p,q}(U) \longrightarrow \mathscr{D}_{X,S}^{p,q-1}(V).$$

If $T \in \mathscr{D}_{X,S}^{p,q}(U)$ and $\varphi \in E_c^*(V)$ is a test form, then

$$K\rho(T)(\varphi) = (-1)^{p+q} T(\rho K(\varphi)).$$

Hence, using that $\bar{\partial} K(\varphi) + K(\bar{\partial}\varphi) = \varphi$, and that $\varphi = \rho\varphi$, we have

$$(\bar{\partial} K\rho T + K\rho\bar{\partial} T + T)(\varphi) = -T(\bar{\partial}(\rho) \wedge K(\varphi)).$$

Observe that, even if the support of φ is contained in V, the support of $K(\varphi)$ can be $\mathbb{C}^n$; therefore the right hand side of the above equation may be non zero.
We compute

$$\begin{aligned} T(\bar{\partial}(\rho) \wedge K(\varphi)) &= T\left(\bar{\partial}(\rho) \wedge \int_{w\in\mathbb{C}^n} k(w,z) \wedge \varphi(w)\right) \\ &= T\left(\int_{w\in\mathbb{C}^n} \bar{\partial}(\rho) \wedge k(w,z) \wedge \varphi(w)\right). \end{aligned}$$

Since $\operatorname{supp}(\varphi) \subset V$ and $\bar{\partial}(\rho)|_V \equiv 0$, we can find a number $\epsilon > 0$ such that, if $\|z - w\| < \epsilon$, then $\bar{\partial}(\rho) \wedge k(w,z) \wedge \varphi(w) = 0$. Since the singularities of $k(w,z)$ are concentrated on the diagonal, it follows that the differential form $\bar{\partial}(\rho) \wedge k(w,z) \wedge \varphi(w)$ is smooth. Therefore, the current in V given by

$$\varphi \longmapsto T\left(\int_{w\in\mathbb{C}^n} \bar{\partial}(\rho) \wedge k(w,z) \wedge \varphi(w)\right),$$

is the current associated to the smooth differential form $T_z\left(\bar{\partial}(\rho)\wedge k(w,z)\right)$, where the subindex z means that T only acts on the z variable, being $w\in V$ a parameter. This smooth form will be denoted by $\Psi(T)$.
Summing up, we have shown that, for any current $T\in \mathscr{D}^{p,q}_{X,S}(U)$ there exists a smooth differential form $\Psi(T)\in \mathscr{E}^{p,q}_X(V)$ such that

$$T\mid_V = -\bar{\partial}K\rho T - K\rho\bar{\partial}T - \Psi(T).$$

Observe that we can not say that Ψ is a quasi-inverse of ι_x because it depends on the choice of ρ and it is not possible to choose a single ρ that can be applied to all T. Hence it is not a well defined operator at the level of stalks. Let now $T\in \mathscr{D}^{p,*}_{X,S,x}$ be closed. It is defined in some neighborhood of x, say U'. Applying the above procedure we find a smooth differential form $\Psi(T)$ defined on a relatively compact subset of U', say V', that is cohomologous to T. Hence the map induced by ι_x in cohomology is surjective. Let $\omega\in \mathscr{E}^{p,*}_{X,x}$ be closed and such that $\iota_x\omega=\bar{\partial}T$ for some $T\in \mathscr{D}^{p,*-1}_{X,S,x}$. We may assume that ω and T are defined is some neighborhood U'' of x. Then, on some relatively compact subset $V''\subset U''$, we have

$$\omega\mid_{V''} = \bar{\partial}T\mid_{V''} = -\bar{\partial}K\rho\omega - \bar{\partial}\Psi(T).$$

Since $K\rho\omega$ and $\Psi(T)$ are smooth differential forms we conclude that the map induced by ι_x in cohomology is injective. □

We will denote by $\mathcal{D}^*_D(X,S,p)$ the Deligne complex associated to $D^*(X,S)$. The following two results are direct consequences of theorem 4.5.

Corollary 4.6. *The inclusion $\mathcal{D}^*_D(X,S,p)\longrightarrow \mathcal{D}^*_D(X,p)$ induces an isomorphism*

$$H^*(\mathcal{D}^*_D(X,S,p))\cong H^*_{\mathcal{D}^{\text{an}}}(X,\mathbb{R}(p)).$$

Corollary 4.7. *(i) Let $\eta\in\mathcal{D}^n_D(X,p)$ be a current such that*

$$\mathrm{d}_{\mathcal{D}}\,\eta\in\mathcal{D}^{n+1}_D(X,S,p),$$

then there is a current $a\in\mathcal{D}^{n-1}_D(X,p)$ such that $\eta+\mathrm{d}_{\mathcal{D}}\,a\in\mathcal{D}^n_D(X,S,p)$.

(ii) Let $\eta\in\mathcal{D}^n_D(X,S,p)$ be a current such that there is a current $a\in\mathcal{D}^{n-1}_D(X,p)$ with $\eta=\mathrm{d}_{\mathcal{D}}\,a$, then there is a current $b\in\mathcal{D}^{n-1}_D(X,S,p)$ such that $\eta=\mathrm{d}_{\mathcal{D}}\,b$.

□

5 Deformation of resolutions

In this section we will recall the deformation of resolutions based on the Grassmannian graph construction of [1]. We will also recall the Koszul resolution associated to a section of a vector bundle.

The main theme is that given a bounded complex E_* of locally free sheaves (with some properties) on a complex manifold X, one can construct a bounded complex $\operatorname{tr}_1(E_*)_*$ over a certain manifold W. This new manifold has a birational map $\pi\colon W \longrightarrow X\times\mathbb{P}^1$, that is an isomorphism over $X\times\mathbb{P}^1\setminus\{\infty\}$. The complex $\operatorname{tr}_1(E_*)_*$ agrees with the original complex over $X\times\{0\}$ and is particularly simple over $\pi^{-1}(X\times\{\infty\})$. Thus $\operatorname{tr}_1(E_*)_*$ is a deformation of the original complex to a simpler one. The two examples we are interested in are: first, when the original complex is exact, then W agrees with $X\times\mathbb{P}^1$ and $\operatorname{tr}_1(E_*)_*$ was defined in 2.5. Its restriction to $\pi^{-1}(X\times\{\infty\})$ is split; second, when $i\colon Y\longrightarrow X$ is a closed immersion of complex manifolds, and E_* is a bounded resolution of $i_*\mathcal{O}_Y$, then W agrees with the deformation to the normal cone of Y and the restriction of $\operatorname{tr}_1(E_*)_*$ to $\pi^{-1}(X\times\{\infty\})$ is an extension of a Koszul resolution by a split complex. Note that, if we allow singularities, then the Grassmannian graph construction is much more general.

The deformation of resolutions is based on the Grassmannian graph construction of [1], and, in the form that we present here, has been developed in [6] and [20].

In order to fix notations we first recall the deformation to the normal cone and the Koszul resolution associated to the zero section of a vector bundle.

Let $Y\hookrightarrow X$ be a closed immersion of complex manifolds, with Y of pure codimension n. In the sequel we will use notation 2.2. Let $W=W_{Y/X}$ be the blow-up of $X\times\mathbb{P}^1$ along $Y\times\{\infty\}$. Since Y and $X\times\mathbb{P}^1$ are manifolds, W is also a manifold. The map $\pi\colon W\longrightarrow X\times\mathbb{P}^1$ is an isomorphism away from $Y\times\{\infty\}$; we will write P for the exceptional divisor of the blow-up. Then

$$P=\mathbb{P}(N_{Y/X}\otimes N_{\infty/\mathbb{P}^1}^{-1}\oplus\mathbb{C}).$$

Thus P can be seen as the projective completion of the vector bundle $N_{Y/X}\otimes N_{\infty/\mathbb{P}^1}^{-1}$. Note that $N_{\infty/\mathbb{P}^1}$ is trivial although not canonically trivial. Nevertheless we can choose to trivialize it by means of the section $y\in\mathcal{O}_{\mathbb{P}^1}(1)$. Sometimes we will tacitly assume this trivialization and omit $N_{\infty/\mathbb{P}^1}$ from the formulae.

The map $q_W\colon W\longrightarrow\mathbb{P}^1$, obtained by composing π with the projection $q\colon X\times\mathbb{P}^1\longrightarrow\mathbb{P}^1$, is flat and, for $t\in\mathbb{P}^1$, we have

$$q_W^{-1}(t)\cong\begin{cases}X\times\{t\}, & \text{if } t\neq\infty,\\ P\cup\widetilde{X}, & \text{if } t=\infty,\end{cases}$$

where $\widetilde{X}$ is the blow-up of X along Y, and $P\cap\widetilde{X}$ is, at the same time, the divisor at ∞ of P and the exceptional divisor of $\widetilde{X}$.

Following [6] we will use the following notations

$$\begin{array}{ccc} P & \xrightarrow{\ f\ } & W\\ {\scriptstyle\pi_P}\downarrow & & \downarrow{\scriptstyle\pi}\\ Y\times\{\infty\} & \xrightarrow{\ i_\infty\ } & X\times\mathbb{P}^1\end{array}$$

$$\begin{aligned}
i\colon Y &\longrightarrow X, \\
W_\infty &= \pi^{-1}(\infty) = P \cup \widetilde{X}, \\
q\colon X\times\mathbb{P}^1 &\longrightarrow \mathbb{P}^1, && \text{the projection,}\\
p\colon X\times\mathbb{P}^1 &\longrightarrow X, && \text{the projection,}\\
q_W &= q\circ\pi \\
p_W &= p\circ\pi \\
q_Y\colon Y\times\mathbb{P}^1 &\longrightarrow \mathbb{P}^1, && \text{the projection,}\\
p_Y\colon Y\times\mathbb{P}^1 &\longrightarrow Y, && \text{the projection,}\\
j\colon Y\times\mathbb{P}^1 &\longrightarrow W && \text{the induced map,}\\
j_\infty\colon Y\times\{\infty\} &\longrightarrow P.
\end{aligned}$$

Given any map $g\colon Z \longrightarrow X\times\mathbb{P}^1$, we will denote $p_Z = p\circ g$ and $q_Z = q\circ g$. For instance $p_P = p\circ\pi\circ f = p_W\circ f = i\circ\pi_P$, where, in the last equality, we are identifying Y with $Y\times\{\infty\}$.
We next recall the construction of the Koszul resolution. Let Y be a complex manifold and let N be a rank n vector bundle. Let $P=\mathbb{P}(N\oplus\mathbb{C})$ be the projective bundle of lines in $N\oplus\mathbb{C}$. It is obtained by completing N with the divisor at infinity. Let $\pi_P\colon P\longrightarrow Y$ be the projection and let $s\colon Y\longrightarrow P$ be the zero section. On P there is a tautological short exact sequence

$$0\longrightarrow \mathcal{O}(-1)\longrightarrow \pi_P^*(N\oplus\mathbb{C})\longrightarrow Q\longrightarrow 0. \tag{5.1}$$

The above exact sequence and the inclusion $\mathbb{C}\longrightarrow\pi_P^*(N\oplus\mathbb{C})$ induce a section $\sigma\colon\mathcal{O}_P\longrightarrow Q$ that vanishes along the zero section $s(Y)$. By duality we obtain a morphism $Q^\vee\longrightarrow\mathcal{O}_P$ that induces a long exact sequence

$$0\longrightarrow \bigwedge^n Q^\vee\longrightarrow\dots\longrightarrow\bigwedge^1 Q^\vee\longrightarrow\mathcal{O}_P\longrightarrow s_*\mathcal{O}_Y\longrightarrow 0.$$

If F is another vector bundle over Y, we obtain an exact sequence,

$$0\longrightarrow \bigwedge^n Q^\vee\otimes\pi_P^*F\longrightarrow\dots\longrightarrow\bigwedge^1 Q^\vee\otimes\pi_P^*F\longrightarrow\pi_P^*F\longrightarrow s_*F\longrightarrow 0. \tag{5.2}$$

Definition 5.3. The *Koszul resolution* of $s_*(F)$ is the resolution (5.2). The complex

$$0\longrightarrow \bigwedge^n Q^\vee\otimes\pi_P^*F\longrightarrow\dots\longrightarrow\bigwedge^1 Q^\vee\otimes\pi_P^*F\longrightarrow\pi_P^*F\longrightarrow 0$$

will be denoted by $K(F,N)$. When $\overline{N}$ is a hermitian vector bundle, the exact sequence (5.1) induces a hermitian metric on Q. If, moreover, $\overline{F}$ is also a hermitian vector bundle, all the vector bundles that appear in the Koszul resolution have an induced hermitian metric. We will denote by $K(\overline{F},\overline{N})$ the corresponding complex of hermitian vector bundles.

In particular, we shall write $K(\overline{\mathcal{O}_Y},\overline{N})$ if $F=\mathcal{O}_Y$ is endowed with the trivial metric $\|1\|=1$, unless expressly stated otherwise.

We finish this section by recalling the results about deformation of resolutions that will be used in the sequel. For more details see [1] II.1, [6] Section 4 (c) and [20] Section 1.

Theorem 5.4. *Let $i : Y \hookrightarrow X$ be a closed immersion of complex manifolds, where Y may be empty. Let $U = X \setminus Y$. Let F be a vector bundle over Y and $E_* \longrightarrow i_*F \longrightarrow 0$ be a resolution of i_*F. Then there exists a complex manifold $W = W(E_*)$, called the Grassmannian graph construction, with a birational map $\pi \colon W \longrightarrow X \times \mathbb{P}^1$ and a complex of vector bundles, $\mathrm{tr}_1(E_*)_*$, over W such that*

(i) The map π is an isomorphism away from $Y \times \{\infty\}$. The restriction of $\mathrm{tr}_1(E_*)_*$ to $X \times (\mathbb{P}^1 \setminus \{\infty\})$ is isomorphic to $p_W^* E_*$ restricted to $X \times (\mathbb{P}^1 \setminus \{\infty\})$. Moreover, If $\widetilde{X}$ is the Zariski closure of $U \times \{\infty\}$ inside W, the restriction of $\mathrm{tr}_1(E_*)_*$ to $\widetilde{X}$ is split acyclic. In particular, if Y is empty or F is the zero vector bundle, hence E_* is acyclic in the whole X, then $W = X \times \mathbb{P}^1$ and $\mathrm{tr}_1(E_*)_*$ is the first transgression exact sequence introduced in 2.5.

(ii) When Y is non-empty and F is a non-zero vector bundle over Y, then $W(E_*)$ agrees with $W_{Y/X}$, the deformation to the normal cone of Y. Moreover, there is an exact sequence of resolutions on P

$$\begin{array}{ccccccccc} 0 & \longrightarrow & A_* & \longrightarrow & \mathrm{tr}_1(E_*)_* \mid_P & \longrightarrow & K(F, N_{Y/X} \otimes N_{\infty/\mathbb{P}^1}^{-1}) & \longrightarrow & 0\ , \\ & & \downarrow & & \downarrow & & \downarrow & & \\ & & 0 & \longrightarrow & (j_\infty)_*F & \xrightarrow{=} & (j_\infty)_*F & & \end{array}$$

where A_* is split acyclic and $K(F, N_{Y/X} \otimes N_{\infty/\mathbb{P}^1}^{-1})$ is the Koszul resolution.

(iii) Let $f \colon X' \longrightarrow X$ be a morphism of complex manifolds and assume that we are in one of the following cases:

(a) The map f is smooth.

(b) The map f is arbitrary and E_* is acyclic.

(c) f is transverse to Y.

Then $E'_* := f^*(E_*)$ is exact over $f^{-1}(U)$,

$$W' := W(E'_*) = W \underset{X}{\times} X',$$

with $f_W \colon W' \longrightarrow W$ the induced map, and we have $f_W^*(\mathrm{tr}_1(E_*)_*) = \mathrm{tr}_1(f^*(E_*))_*$.

(iv) *If the vector bundles E_i are provided with hermitian metrics, then one can choose a hermitian metric on* $\operatorname{tr}_1(E_*)_*$ *such that its restriction to* $X \times \{0\}$ *is isometric to* E_* *and the restriction to* $U \times \{\infty\}$ *is orthogonally split. We will denote by* $\operatorname{tr}_1(\overline{E}_*)_*$ *the complex* $\operatorname{tr}_1(E_*)_*$ *with such a choice of hermitian metrics. Moreover, this choice of metrics can be made functorial. That is, if* f *is a map as in item (iii), then*

$$f_W^*(\operatorname{tr}_1(\overline{E}_*)_*) = \operatorname{tr}_1(f^*(\overline{E}_*))_*$$

Proof. The case when E_* is acyclic has already been treated. For the case when Y is non-empty and F is non zero, we first recall the construction of the Grassmannian graph of an arbitrary complex from [20], which is more general than what we need here. If E is a vector bundle over X we will denote by $E(i)$ the vector bundle over $X \times \mathbb{P}^1$ given by $E(i) = p^*E \otimes q^*\mathcal{O}(i)$.

Let $\widetilde{C}_*$ be the complex of locally free sheaves given by $\widetilde{C}_i = E_i(i) \oplus E_{i-1}(i-1)$ with differential given by $\mathrm{d}(a,b) = (b,0)$. On $X \times (\mathbb{P}^1 \setminus \{\infty\})$ we consider, for each i, the inclusion of vector bundles $\gamma_i \colon E_i \hookrightarrow \widetilde{C}_i$ given by $s \longmapsto (s \otimes y^i, \mathrm{d}\, s \otimes y^{i-1})$. Let G be the product of the Grassmann bundles $Gr(n_i, \widetilde{C}_i)$ that parametrize rank $n_i = \operatorname{rk} E_i$ subbundles of $\widetilde{C}_i$ over $X \times \mathbb{P}^1$. The inclusion $\gamma_* \colon \bigoplus E_i \longrightarrow \bigoplus \widetilde{C}_i$ induces a section s of G over $X \times \mathbb{A}^1$.

Then $W(E_*)$ is defined to be the closure of $s(X \times \mathbb{A}^1)$ in G. Since the projection from G to $X \times \mathbb{P}^1$ is proper, the same is true for the induced map $\pi \colon W \longrightarrow X \times \mathbb{P}^1$. For each i, the induced map $W \longrightarrow Gr(n_i, \widetilde{C}_i)$ defines a subbundle $\operatorname{tr}_1(E_*)_i$ of $\pi^*\widetilde{C}_i$. This subbundle agrees with E_i over $X \times \mathbb{A}^1$. The differential of $\widetilde{C}_*$ induces a differential on $\operatorname{tr}_1(E_*)_*$.

Assume now that the bundles E_i are provided with hermitian metrics. Using the Fubini-Study metric of $\mathcal{O}(1)$ we obtain induced metrics on $\widetilde{C}_i$. Over $\pi^{-1}(X \times (\mathbb{P}^1 \setminus \{\infty\}))$ we induce a metric on $\operatorname{tr}_1(E_*)_i$ by means of the identification with E_i. Over $\pi^{-1}(X \times (\mathbb{P}^1 \setminus \{0\}))$ we consider on $\operatorname{tr}_1(E_*)_i$ the metric induced by $\widetilde{C}_i$. We glue together both metrics with the partition of unity $\{\sigma_0, \sigma_\infty\}$ of notation 2.2.

In the case we are interested there is a more explicit description of $\operatorname{tr}_1(E_*)_*$ given in [6] Section 4 (c). Namely, $\operatorname{tr}_1(E_*)_i$ is the kernel of the morphism

$$\phi \colon p_W^*\widetilde{C}_i = p_W^*E_i(i) \oplus p_W^*E_{i-1}(i-1) \longrightarrow p_W^*E_{i-1}(i) \oplus p_W^*E_{i-2}(i-1) \quad (5.5)$$

given by $\phi(s,t) = (\mathrm{d}\, s - t \otimes y, \mathrm{d}\, t)$.

The only statements that are not explicitly proved in [6] Section 4 (c) or [20] Section 1 are the functoriality when f is not smooth and the properties of the explicit choice of metrics.

If the complex E_* is acyclic, then the same is true for $E'_* = f^*E_*$. In this case $W = X \times \mathbb{P}^1$ and $W' = X' \times \mathbb{P}^1$. Then the functoriality follows from the definition of $\operatorname{tr}_1(E_*)_*$.

Assume now that we are in case (iii)c. We can form the Cartesian square

$$\begin{array}{ccc} Y' & \xrightarrow{i'} & X' \\ {\scriptstyle g}\downarrow & & \downarrow{\scriptstyle f} \\ Y & \xrightarrow{i} & X \end{array}$$

where i' is also a closed immersion of complex manifolds. Then we have that E'_* is a resolution of $i'_* g^* F$. Hence $W' = W(E'_*)$ is the deformation to the normal cone of Y' and therefore $W' = W \underset{X}{\times} X'$. Again the functoriality of $\operatorname{tr}_1(E_*)_*$ can be checked using the explicit construction of [20] Section 1 that we have recalled above. □

Remark 5.6. (i) The definition of $\operatorname{tr}_1(E_*)$ can be extended to any bounded chain complex over a integral scheme (see [20]).

(ii) There is a sign difference in the definition of the inclusion γ used in [20] and the one used in [6]. We have followed the signs of the first reference.

6 Singular Bott-Chern classes

Throughout this section we will use notation 1.3. In particular we will write

$$\widetilde{\mathcal{D}}^n_D(X,p) = \mathcal{D}^n_D(X,p)/\operatorname{d}_{\mathcal{D}} \mathcal{D}^{n-1}_D(X,p),$$
$$\widetilde{\mathcal{D}}^n_D(X,S,p) = \mathcal{D}^n_D(X,S,p)/\operatorname{d}_{\mathcal{D}} \mathcal{D}^{n-1}_D(X,S,p).$$

A particularly important current is $W_1 \in \mathcal{D}^1_D(\mathbb{P}^1, 1)$ given by

$$W_1 = [\frac{-1}{2} \log \|t\|^2]. \tag{6.1}$$

With the above convention, this means that

$$W_1(\eta) = \frac{1}{2\pi i} \int_{\mathbb{P}^1} \frac{-1}{2} \log \|t\|^2 \bullet \eta. \tag{6.2}$$

By the Poincaré-Lelong equation

$$\operatorname{d}_{\mathcal{D}} W_1 = \delta_\infty - \delta_0. \tag{6.3}$$

Note that the current W_1 was used in the construction of Bott-Chern classes (definition 2.11) and will also have a role in the definition of singular Bott-Chern classes.

Before defining singular Bott-Chern classes we need to define the objects that give rise to them.

Definition 6.4. Let $i\colon Y \longrightarrow X$ be a closed immersion of complex manifolds. Let N be the normal bundle of Y and let h_N be a hermitian metric on N. We denote $\overline{N} = (N, h_N)$. Let r_N be the rank of N, that agrees with the codimension of Y in X. Let $\overline{F} = (F, h_F)$ be a hermitian vector bundle on Y of rank r_F. Let $\overline{E}_* \to i_*F$ be a metric on the coherent sheaf i_*F. The four-tuple

$$\overline{\xi} = (i, \overline{N}, \overline{F}, \overline{E}_*). \tag{6.5}$$

is called a *hermitian embedded vector bundle*. The number r_F will be called the *rank* of $\overline{\xi}$ and the number r_N will be called the *codimension* of $\overline{\xi}$.
By convention, any exact complex of hermitian vector bundles on X will be considered a hermitian embedded vector bundle of any rank and codimension.

Obviously, to any hermitian embedded vector bundle we can associate the metrized coherent sheaf $(i_*F, \overline{E}_* \to i_*F)$.

Definition 6.6. A *singular Bott-Chern class* for a hermitian embedded vector bundle $\overline{\xi}$ is a class $\widetilde{\eta} \in \bigoplus_p \widetilde{\mathcal{D}}_D^{2p-1}(X, p)$ such that

$$\mathrm{d}_{\mathcal{D}}\, \eta = \sum_{i=0}^{n} (-1)^i [\mathrm{ch}(\overline{E}_i)] - i_*([\mathrm{Td}^{-1}(\overline{N})\, \mathrm{ch}(\overline{F})]) \tag{6.7}$$

for any current $\eta \in \tilde{\eta}$.

The existence of this class is guaranteed by the Grothendieck-Riemann-Roch theorem, which implies that the two currents in the right hand side of equation (6.7) are cohomologous.
Even if we have defined singular Bott-Chern classes as classes of currents with arbitrary singularities, it is an important observation that in each singular Bott-Chern class we can find representatives with controlled singularities. Let $N^*_{Y,0}$ be the conormal bundle of Y with the zero section deleted. It is a closed conical subset of $T^*_0(X)$. Since the current

$$\sum_{i=0}^{n} (-1)^i [\mathrm{ch}(\overline{E}_i)] - i_*([\mathrm{Td}^{-1}(\overline{N})\, \mathrm{ch}(\overline{F})]) \\ = \sum_{i=0}^{n} (-1)^i [\mathrm{ch}(\overline{E}_i)] - \mathrm{Td}^{-1}(\overline{N})\, \mathrm{ch}(\overline{F}) \delta_Y$$

belongs to $\mathcal{D}^*_D(X, N^*_{Y,0}, p)$, by corollary 4.7, we obtain

Proposition 6.8. *Let $\overline{\xi} = (i, \overline{N}, \overline{F}, \overline{E}_*)$ be a hermitian embedded vector bundle as before. Then any singular Bott-Chern class for $\overline{\xi}$ belongs to the subset*

$$\bigoplus_p \widetilde{\mathcal{D}}_D^{2p-1}(X, N^*_{Y,0}, p) \subset \bigoplus_p \widetilde{\mathcal{D}}_D^{2p-1}(X, p).$$

□

This result will allow us to define inverse images of singular Bott-Chern classes for certain maps.
Let $f\colon X' \longrightarrow X$ be a morphism of complex manifolds that is transverse to Y. We form the Cartesian square

$$\begin{array}{ccc} Y' & \xrightarrow{i'} & X' \\ \Big\downarrow{\scriptstyle g} & & \Big\downarrow{\scriptstyle f} \\ Y & \xrightarrow{i} & X \end{array} .$$

Observe that, by the transversality hypothesis, the normal bundle to Y' on X' is the inverse image of the normal bundle to Y on X and f^*E_* is a resolution of i'_*g^*F. Thus we write $f^*\overline{\xi} = (i', f^*\overline{N}, g^*\overline{F}, f^*\overline{E}_*)$, which is a hermitian embedded vector bundle.
By proposition 6.8, given any singular Bott-Chern class $\widetilde{\eta}$ for ξ, we can find a representative $\eta \in \bigoplus_p \mathcal{D}_D^{2p-1}(X, N^*_{Y,0}, p)$. By theorem 4.3, there is a well defined current $f^*\eta$ and it is a singular Bott-Chern current for $f^*\xi$. Therefore we can define $f^*(\widetilde{\eta}) = \widetilde{f^*(\eta)}$. Again by theorem 4.3, this class does not depend on the choice of the representative η.
Our next objective is to study the possible definitions of functorial singular Bott-Chern classes.

Definition 6.9. Let r_F and r_N be two integers. A *theory of singular Bott-Chern classes of rank r_F and codimension r_N* is an assignment which, to each hermitian embedded vector bundle $\overline{\xi} = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_*)$ of rank r_F and codimension r_N, assigns a class of currents

$$T(\overline{\xi}) \in \bigoplus_p \widetilde{\mathcal{D}}_D^{2p-1}(X,p)$$

satisfying the following properties

(i) (Differential equation) The following equality holds

$$\mathrm{d}_{\mathcal{D}}\, T(\overline{\xi}) = \sum_i (-1)^i [\mathrm{ch}(\overline{E}_i)] - i_*([\mathrm{Td}^{-1}(\overline{N})\,\mathrm{ch}(\overline{F})]). \tag{6.10}$$

(ii) (Functoriality) For every morphism $f\colon X' \longrightarrow X$ of complex manifolds that is transverse to Y, then

$$f^*T(\overline{\xi}) = T(f^*\overline{\xi}).$$

(iii) (Normalization) Let $\overline{A} = (A_*, g_*)$ be a non-negatively graded orthogonally split complex of vector bundles. Write $\overline{\xi} \oplus \overline{A} = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_* \oplus \overline{A}_*)$. Then $T(\overline{\xi}) = T(\overline{\xi} \oplus \overline{A})$. Moreover, if $X = \operatorname{Spec}\mathbb{C}$ is one point, $Y = \emptyset$ and $\overline{E}_* = 0$, then $T(\overline{\xi}) = 0$.

A *theory of singular Bott-Chern classes* is an assignment as before, for all positive integers r_F and r_M. When the inclusion i and the bundles F and N are clear from the context, we will denote $T(\overline{\xi})$ by $T(\overline{E}_*)$. Sometimes we will have to restrict ourselves to complex algebraic manifolds and algebraic vector bundles. In this case we will talk of *theory of singular Bott-Chern classes for algebraic vector bundles*.

Remark 6.11. (i) Recall that the case when $Y=\emptyset$ and $\overline{E}_*$ is any bounded exact sequence of hermitian vector bundles is considered a hermitian embedded vector bundle of arbitrary rank. In this case, the properties above imply that

$$T(\overline{\xi})=[\widetilde{\mathrm{ch}}(\overline{E}_*)],$$

where $\widetilde{\mathrm{ch}}$ is the Bott-Chern class associated to the Chern character. That is, for acyclic complexes, any theory of singular Bott-Chern classes agrees with the Bott-Chern classes associated to the Chern character.

(ii) If the map f is transverse to Y, then either $f^{-1}(Y)$ is empty or it has the same codimension as Y. Moreover, it is clear that f^*F has the same rank as F. Therefore, the properties of singular Bott-Chern classes do not mix rank or codimension. This is why we have defined singular Bott-Chern classes for a particular rank and codimension.

(iii) By contrast with the case of Bott-Chern classes, the properties above are not enough to characterize singular Bott-Chern classes.

For the rest of this section we will assume the existence of a theory of singular Bott-Chern classes and we will obtain some consequences of the definition.
We start with the compatibility of singular Bott-Chern classes with exact sequences and Bott-Chern classes.
Let

$$\overline{\chi}\colon 0\longrightarrow \overline{F}_n\longrightarrow \dots\longrightarrow \overline{F}_1\longrightarrow \overline{F}_0\longrightarrow 0 \tag{6.12}$$

be a bounded exact sequence of hermitian vector bundles on Y. For $j=0,\dots,n$, let $\overline{E}_{j,*}\longrightarrow i_*F_j$ be a resolution, and assume that they fit in a commutative diagram

$$\begin{array}{ccccccccccc} 0 & \longrightarrow & \overline{E}_{n,*} & \longrightarrow & \cdots & \longrightarrow & \overline{E}_{1,*} & \longrightarrow & \overline{E}_{0,*} & \longrightarrow & 0\ , \\ & & \downarrow & & & & \downarrow & & \downarrow & & \\ 0 & \longrightarrow & i_*F_n & \longrightarrow & \cdots & \longrightarrow & i_*F_1 & \longrightarrow & i_*F_0 & \longrightarrow & 0 \end{array}$$

with exact rows. We write $\overline{\xi_j}=(i\colon Y\longrightarrow X,\overline{N},\overline{F}_j,\overline{E}_{j,*})$. For each k, we denote by $\overline{\eta}_k$ the exact sequence

$$0\longrightarrow \overline{E}_{n,k}\longrightarrow \dots\longrightarrow \overline{E}_{1,k}\longrightarrow \overline{E}_{0,k}\longrightarrow 0.$$

Proposition 6.13. *With the above notations, the following equation holds:*

$$T(\bigoplus_{j\ even} \overline{\xi}_j) - T(\bigoplus_{j\ odd} \overline{\xi}_j) = \sum_k (-1)^k [\widetilde{\mathrm{ch}}(\overline{\eta}_k)] - i_*([\mathrm{Td}^{-1}(\overline{N})\widetilde{\mathrm{ch}}(\overline{\chi})]).$$

Here the direct sum of hermitian embedded vector bundles, involving the same embedding and the same hermitian normal bundle, is defined in the obvious manner.

Proof. We consider the construction of theorem 5.4 for each of the exact sequences $\overline{\eta}_k$ and the exact sequence $\overline{\chi}$. For each k, we have $W_X := W(\overline{\eta}_k) = X \times \mathbb{P}^1$ and we denote $W_Y := W(\overline{\chi}) = Y \times \mathbb{P}^1$. On W_Y we consider the transgression exact sequence $\mathrm{tr}_1(\overline{\chi})_*$ and on W_X we consider the transgression exact sequences $\mathrm{tr}_1(\overline{\eta_k})_*$. We denote by $j\colon W_Y \longrightarrow W_X$ the induced morphism. Then there is an exact sequence (of exact sequences)

$$\dots \longrightarrow \mathrm{tr}_1(\overline{\eta}_1)_* \longrightarrow \mathrm{tr}_1(\overline{\eta}_0)_* \longrightarrow j_* \mathrm{tr}_1(\overline{\chi})_* \longrightarrow 0.$$

We denote

$$\mathrm{tr}_1(\overline{\chi})_+ = \bigoplus_{j \text{ even}} \mathrm{tr}_1(\overline{\chi})_j, \qquad \mathrm{tr}_1(\overline{\chi})_- = \bigoplus_{j \text{ odd}} \mathrm{tr}_1(\overline{\chi})_j,$$
$$\mathrm{tr}_1(\overline{\eta}_k)_+ = \bigoplus_{j \text{ even}} \mathrm{tr}_1(\overline{\eta}_k)_j, \quad \mathrm{tr}_1(\overline{\eta}_k)_- = \bigoplus_{j \text{ odd}} \mathrm{tr}_1(\overline{\eta}_k)_j,$$

and

$$\mathrm{tr}_1(\overline{\xi})_+ = (j\colon W_Y \longrightarrow W_X, p_Y^*\overline{N}, \mathrm{tr}_1(\overline{\chi})_+, \mathrm{tr}_1(\overline{\eta}_*)_+),$$
$$\mathrm{tr}_1(\overline{\xi})_- = (j\colon W_Y \longrightarrow W_X, p_Y^*\overline{N}, \mathrm{tr}_1(\overline{\chi})_-, \mathrm{tr}_1(\overline{\eta}_*)_-),$$

where here $p_Y\colon W_Y \longrightarrow Y$ denotes the projection.
We consider the current on $X \times \mathbb{P}^1$ given by $W_1 \bullet \big(T(\mathrm{tr}_1(\overline{\xi})_+) - T(\mathrm{tr}_1(\overline{\xi})_-)\big)$. This current is well defined because the wave front set of W_1 is the conormal bundle of $(X \times \{0\}) \cup (X \times \{\infty\})$, whereas the wave front set of $T(\mathrm{tr}_1(\overline{\xi})_\pm)$ is the conormal bundle of $Y \times \mathbb{P}^1$.
By the functoriality of the transgression exact sequences, we obtain that

$$\mathrm{tr}_1(\overline{\xi})_+ \mid_{X\times\{0\}} = \bigoplus_{j \text{ even}} \overline{\xi}_j, \quad \mathrm{tr}_1(\overline{\xi})_- \mid_{X\times\{0\}} = \bigoplus_{j \text{ odd}} \overline{\xi}_j.$$

Moreover, using the fact that, for any bounded acyclic complex of hermitian vector bundles $\overline{E}_*$, the exact sequence $\mathrm{tr}_1(\overline{E}_*) \mid_{X\times\{\infty\}}$ is orthogonally split, we have an isometry

$$\mathrm{tr}_1(\overline{\xi})_+ \mid_{X\times\{\infty\}} \cong \mathrm{tr}_1(\overline{\xi})_- \mid_{X\times\{\infty\}} .$$

We now denote by $p_X\colon W_X \longrightarrow X$ the projection. Using the properties that define a theory of singular Bott-Chern classes, in the group $\bigoplus_p \widetilde{\mathcal{D}}_D^{2p-1}(X, N^*_{Y,0}, p)$, the following holds

$$\begin{aligned}
0 &= \mathrm{d}_{\mathcal{D}}(p_X)_* \left(W_1 \bullet T(\operatorname{tr}_1(\overline{\xi})_+) - W_1 \bullet T(\operatorname{tr}_1(\overline{\xi})_-)\right) \\
&= \left(T(\operatorname{tr}_1(\overline{\xi})_+) - T(\operatorname{tr}_1(\overline{\xi})_-)\right) |_{X\times\{\infty\}} - \left(T(\operatorname{tr}_1(\overline{\xi})_+) - T(\operatorname{tr}_1(\overline{\xi})_-)\right) |_{X\times\{0\}} \\
&- (p_X)_* \sum_k (-1)^k W_1 \bullet (\operatorname{ch}(\operatorname{tr}_1(\overline{\eta}_k)_+) - \operatorname{ch}(\operatorname{tr}_1(\overline{\eta}_k)_-)) \\
&+ (p_X)_* \left(W_1 \bullet j_* \left[\operatorname{Td}^{-1}(p_Y^* \overline{N}) \operatorname{ch}(\operatorname{tr}_1(\overline{\chi})_+) - \operatorname{Td}^{-1}(p_Y^* \overline{N}) \operatorname{ch}(\operatorname{tr}_1(\overline{\chi})_-)\right]\right) \\
&= -T(\bigoplus_{j \text{ even}} \overline{\xi}_j) + T(\bigoplus_{j \text{ odd}} \overline{\xi}_j) + \sum (-1)^k [\widetilde{\operatorname{ch}}(\overline{\eta}_k)] - i_*[\operatorname{Td}^{-1}(\overline{N}) \bullet \widetilde{\operatorname{ch}}(\overline{\chi})],
\end{aligned}$$

which implies the proposition. □

The following result is a consequence of proposition 6.13 and theorem 2.24.

Corollary 6.14. *Let $Y \longrightarrow X$ be a closed immersion of complex manifolds. Let $\overline{\chi}$ be an exact sequence of hermitian vector bundles on Y as* (6.12)*. For each j, let $\xi_j = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}_j, \overline{E}_{j,*})$ be a hermitian embedded vector bundle. We denote by $\overline{\varepsilon}$ the induced exact sequence of metrized coherent sheaves. Then*

$$T(\bigoplus_{j \text{ even}} \overline{\xi}_j) - T(\bigoplus_{j \text{ odd}} \overline{\xi}_j) = [\widetilde{\operatorname{ch}}(\overline{\varepsilon})] - i_*([\operatorname{Td}^{-1}(\overline{N})\widetilde{\operatorname{ch}}(\overline{\chi})]).$$

□

We now study the effect of changing the metric of the normal bundle N.

Proposition 6.15. *Let $\overline{\xi}_0 = (i, \overline{N}_0, \overline{F}, \overline{E}_*)$ be a hermitian embedded vector bundle, where $\overline{N}_0 = (N, h_0)$. Let h_1 be another metric in the vector bundle N and write $\overline{N}_1 = (N, h_1)$, $\overline{\xi}_1 = (i, \overline{N}_1, \overline{F}, \overline{E}_*)$. Then*

$$T(\overline{\xi}_0) - T(\overline{\xi}_1) = -i_*[\widetilde{\operatorname{Td}^{-1}}(N, h_0, h_1) \operatorname{ch}(\overline{F})].$$

Proof. The proof is completely analogous to the proof of proposition 6.13. □

We now study the case when Y is the zero section of a completed vector bundle. Let $\overline{F}$ and $\overline{N}$ be hermitian vector bundles over Y. We denote $P = \mathbb{P}(N \oplus \mathbb{C})$, the projective bundle of lines in $N \oplus \mathcal{O}_Y$. Let $s\colon Y \longrightarrow P$ denote the zero section and let $\pi_P\colon P \longrightarrow Y$ denote the projection. Let $K(\overline{F}, \overline{N})$ be the Koszul resolution of definition 5.3. We will use the notations before this definition. The following result is due to Bismut, Gillet and Soulé for the particular choice of singular Bott-Chern classes defined in [6].

Theorem 6.16. *Let T be a theory of singular Bott-Chern classes of rank r_F and codimension r_N. Let Y be a complex manifold and let $\overline{F}$ and $\overline{N}$ be hermitian vector bundles of rank r_F and r_N respectively. Then the current $(\pi_P)_*(T(K(\overline{F}, \overline{N})))$ is closed. Moreover the cohomology class that it represents does not depend on the metric of N and F and determines a characteristic class for pairs of vector bundles of rank r_F and r_N. We denote this class by $C_T(F, N)$.*

Proof. We have that

$$\begin{aligned}
&\mathrm{d}_{\mathcal{D}}(\pi_P)_*(T(K(\overline{F},\overline{N})))\\
&\qquad=(\pi_P)_*(\mathrm{d}_{\mathcal{D}}\,T(K(\overline{F},\overline{N})))\\
&\qquad=(\pi_P)_*\left(\sum_{k=0}^{r}(-1)^k[\operatorname{ch}(\bigwedge^k\overline{Q}^{\vee})\pi_P^*\operatorname{ch}(\overline{F})]-s_*[\operatorname{Td}^{-1}(\overline{N})\operatorname{ch}(\overline{F})]\right)\\
&\qquad=\big((\pi_P)_*[c_r(\overline{Q})\operatorname{Td}^{-1}(\overline{Q})]-[\operatorname{Td}^{-1}(\overline{N})]\big)\operatorname{ch}(\overline{F})).
\end{aligned}$$

Therefore, the fact that the current $(\pi_P)_*(T(K(\overline{F},\overline{N})))$ is closed follows from corollary 3.8. The fact that this class is functorial on $(Y,\overline{N},\overline{F})$ is clear from the construction Thus, the fact that it does not depend on the hermitian metrics of N and F follows from proposition 1.7. □

Remark 6.17. By theorem 1.8 we know that, if we restrict ourselves to the algebraic category, $C_T(F,N)$ is given by a power series on the Chern classes with coefficients in $\mathbb{D}$. By degree reasons

$$C_T(F,N)\in\bigoplus_p H^{2p-1}_{\mathcal{D}^{\mathrm{an}}}(Y,\mathbb{R}(p)).$$

Let $\mathbf{1}_1\in H^1_{\mathcal{D}}(*,\mathbb{R}(1))$ be the element determined by the constant function with value 1 in $\mathcal{D}^1(*,1)$. Then $C_T(F,N)/\mathbf{1}_1$ is a power series in the Chern classes of N and F with real coefficients.

7 Classification of theories of singular Bott-Chern classes

The aim of this section is to give a complete classification of the possible theories of singular Bott-Chern classes. This classification is given in terms of the characteristic class C_T introduced in the previous section.

Theorem 7.1. *Let r_F and r_N be two positive integers. Let C be a characteristic class for pairs of vector bundles of rank r_F and r_N. Then there exists a unique theory T_C of singular Bott-Chern classes of rank r_F and codimension r_N such that $C_{T_C}=C$.*

Proof. We first prove the uniqueness. Assume that T is a theory of singular Bott-Chern classes such that $C_T=C$. Let $\overline{\xi}=(i\colon Y\longrightarrow X,\overline{N},\overline{F},\overline{E}_*)$ be a hermitian embedded vector bundle as in section 6. Let W be the deformation to the normal cone of Y. We will use all the notations of section 5. In particular, we will denote by $p_{\widetilde{X}}\colon\widetilde{X}\longrightarrow X$ and $p_P\colon P\longrightarrow X$ the morphisms induced by restricting p_W. Recall that p_P can be factored as

$$P\xrightarrow{\pi_P}Y\xrightarrow{i}X.$$

The normal vector bundle to the inclusion $j\colon Y\times\mathbb{P}^1\longrightarrow W$ is isomorphic to $p_Y^*N\otimes q_Y^*\mathcal{O}(-1)$. We provide it with the hermitian metric induced by the metric of N and the Fubini-Study metric of $\mathcal{O}(-1)$ and we denote it by $\overline{N}'$.

By theorem 5.4 we have a complex of hermitian vector bundles, $\operatorname{tr}_1(E_*)_*$ such that the restriction $\operatorname{tr}_1(E_*)_*|_{X\times\{0\}}$ is isometric to E_*, the restriction $\operatorname{tr}_1(E_*)_*|_{\widetilde{X}}$ is orthogonally split and there is an exact sequence on P

$$0 \longrightarrow A_* \longrightarrow \operatorname{tr}_1(E_*)_*|_P \longrightarrow K(F,N) \longrightarrow 0,$$

where A_* is split acyclic and $K(F,N)$ is the Koszul resolution. Recall that we have trivialized $N^{-1}_{\infty/\mathbb{P}^1}$ by means of the section y of $\mathcal{O}_{\mathbb{P}^1}(1)$. We choose a hermitian metric in every bundle of A_* such that it becomes orthogonally split. For each k we will denote by $\overline{\eta}_k$ the exact sequence of hermitian vector bundles

$$0 \longrightarrow \overline{A}_k \longrightarrow \operatorname{tr}_1(\overline{E}_*)_k|_P \longrightarrow K(\overline{F},\overline{N})_k \longrightarrow 0. \tag{7.2}$$

Observe that the current W_1 is defined as the current associated to a locally integrable differential form. The pull-back of this form to W is also locally integrable. Therefore it defines a current on W that we also denote by W_1. Moreover, since the wave front sets of W_1 and of $T(\operatorname{tr}_1(\overline{E}_*)_*)$ are disjoint, there is a well defined current $W_1 \bullet T(\operatorname{tr}_1(\overline{E}_*)_*)$. Then, using the properties of singular Bott-Chern classes in definition 6.9, the equality

$$\begin{aligned}0 &= \mathrm{d}_{\mathcal{D}}(p_W)_*\left(W_1 \bullet T(\operatorname{tr}_1(\overline{E}_*)_*)\right)\\ &= (p_{\widetilde{X}})_*(T(\operatorname{tr}_1(\overline{E}_*)_*)|_{\widetilde{X}}) + (p_P)_*(T(\operatorname{tr}_1(\overline{E}_*)_*)|_P) - T(\overline{\xi})\\ &\quad - (p_W)_*\left(W_1 \bullet \left(\sum_k (-1)^k \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_*) - (j_*(\operatorname{ch}(p_Y^*\overline{F})\operatorname{Td}^{-1}(\overline{N}'))\right)\right)\end{aligned}$$

holds in the group $\bigoplus_k \widetilde{\mathcal{D}}^{2k-1}(X,k)$. By properties 6.9(ii) and 6.9(iii), $T(\operatorname{tr}_1(\overline{E}_*)_*)|_{\widetilde{X}} = T(\operatorname{tr}_1(\overline{E}_*)_*|_{\widetilde{X}}) = 0$.
By proposition 6.13 we have

$$T(\operatorname{tr}_1(\overline{E}_*)_*|_P) = T(K(\overline{F},\overline{N})) - \sum_k (-1)^k [\widetilde{\operatorname{ch}}(\overline{\eta}_k)].$$

Moreover, we have

$$(p_P)_*(T(K(\overline{F},\overline{N}))) = i_*(\pi_P)_*(T(K(\overline{F},\overline{N}))) = i_* C_T(F,N).$$

By the definition of N' and the choice of its metric, there are two differential forms a, b on Y, such that

$$\operatorname{ch}(p_Y^*\overline{F})\operatorname{Td}^{-1}(\overline{N}') = p_Y^*(a) + p_Y^*(b) \wedge q_Y^*(c_1(\mathcal{O}(-1))).$$

We denote $\omega = -c_1(\mathcal{O}(-1))$. By the properties of the Fubini-Study metric, ω is invariant under the involution of $\mathbb{P}^1$ that sends t to $1/t$. Then

$$(p_W)_*\left(W_1 \bullet (j_*(\operatorname{ch}(p_Y^*\overline{F})\operatorname{Td}^{-1}(\overline{N}'))\right) = i_*(p_Y)_*(W_1 \bullet (p_Y^* a + p_Y^* b\omega)) = 0$$

because the current W_1 changes sign under the involution $t \longmapsto 1/t$.
Summing up, we have obtained the equation

$$T(\overline{\xi}) = -(p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k) \right) - \sum_k (-1)^k (p_P)_* [\widetilde{\operatorname{ch}}(\overline{\eta}_k)] + i_* C_T(F, N). \quad (7.3)$$

Hence the singular Bott-Chern class is characterized by the properties of definition 6.9 and the characteristic class C_T.
In order to prove the existence of a theory of singular Bott-Chern classes, we use equation (7.3) to define a class $T_C(\xi)$ as follows.

Definition 7.4. Let C be a characteristic class for pairs of vector bundles of rank r_F and r_N as in theorem 7.1. Let $\overline{\xi} = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_*)$ be as in definition 6.9. Let $\overline{A}_*$, $\operatorname{tr}_1(\overline{E}_*)_*$ and $\overline{\eta}_*$ be as in (7.2). Then we define

$$T_C(\overline{\xi}) = -(p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k) \right) - \sum_k (-1)^k (p_P)_* [\widetilde{\operatorname{ch}}(\overline{\eta}_k)] + i_* C(F, N). \quad (7.5)$$

We have to prove that this definition does not depend on the choice of the metric of $\operatorname{tr}_1(\overline{E}_*)_*$ or the metric of $\overline{A}_*$, that T_C satisfies the properties of definition 6.9 and that the characteristic class C_{T_C} agrees with C.
First we prove the independence from the metrics. We denote by h_k the hermitian metric on $\operatorname{tr}_1(\overline{E}_*)_k$ and by g_k the hermitian metric on A_k. Let h'_k and g'_k be another choice of metrics satisfying also that (A_*, g'_*) is orthogonally split, that $(\operatorname{tr}_1(E_*)_k, h'_k)|_{X \times \{0\}}$ is isometric to $\overline{E}_k$ and that $(\operatorname{tr}_1(E_*)_k, h'_k)|_{\widetilde{X}}$ is orthogonally split. We denote by $\overline{\eta}'_k$ the exact sequence η_k provided with the metrics g' and h'. Then, in the group $\bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(X, p)$, we have

$$\begin{aligned} &\sum_k (-1)^k (p_P)_* [\widetilde{\operatorname{ch}}(\overline{\eta}_k)] - \sum_k (-1)^k (p_P)_* [\widetilde{\operatorname{ch}}(\overline{\eta}'_k)] = \\ &\sum_k (-1)^k (p_P)_* \left[\widetilde{\operatorname{ch}}(A_k, g_k, g'_k)\right] - \sum_k (-1)^k (p_P)_* \left[\widetilde{\operatorname{ch}}(\operatorname{tr}_1(E_*)_k|_P, h_k, h'_k)\right]. \end{aligned} \quad (7.6)$$

Observe that the first term of the right hand side vanishes due to the hypothesis of A_* being orthogonally split for both metrics.

Moreover, we also have,

$$(p_W)_*\left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(E_*)_k, h_k)\right) - \\ (p_W)_*\left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(E_*)_k, h'_k)\right) = \\ (p_W)_*\left(\sum_k (-1)^k W_1 \bullet \mathrm{d}_{\mathcal{D}}\, \widetilde{\operatorname{ch}}(\operatorname{tr}_1(E_*)_k, h_k, h'_k)\right). \quad (7.7)$$

But, in the group $\bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(X,p)$,

$$(p_W)_*\left(\sum_k (-1)^k W_1 \bullet \mathrm{d}_{\mathcal{D}}\, \widetilde{\operatorname{ch}}(\operatorname{tr}_1(E_*)_k, h_k, h'_k)\right) = \\ \sum_k (-1)^k (p_{\widetilde{X}})_*[\widetilde{\operatorname{ch}}(\operatorname{tr}_1(E_*)_k, h_k, h'_k)]|_{\widetilde{X}} \\ + \sum_k (-1)^k (p_P)_*[\widetilde{\operatorname{ch}}(\operatorname{tr}_1(E_*)_k, h_k, h'_k)]|_P) \\ - \sum_k (-1)^k [\widetilde{\operatorname{ch}}(\operatorname{tr}_1(E_*)_k, h_k, h'_k)]|_{X\times\{0\}}. \quad (7.8)$$

The last term of the right hand side vanishes because the metrics h_k and h'_k agree when restricted to $X \times \{0\}$ and the first term vanishes by the hypothesis that $\operatorname{tr}_1(E_*)_*|_{\widetilde{X}}$ is orthogonally split with both metrics. Combining equations (7.6), (7.7) and (7.8) we obtain that the right hand side of equation (7.5) does not depend on the choice of metrics.

We next prove the property (i) of definition 6.9. We compute

$$\mathrm{d}_{\mathcal{D}}\, T_C(\overline{\xi}) = -\sum_k (-1)^k \left((p_{\widetilde{X}})_* \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k|_{\widetilde{X}}) + (p_P)_* \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k|_P)\right) \\ + \sum_k (-1)^k \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k|_{X\times\{0\}}) \\ - \sum_k (-1)^k (p_P)_* \left(\operatorname{ch}(\overline{A}_k) + \operatorname{ch}(K(\overline{F},\overline{N})_k) - \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k|_P)\right).$$

Using that $\overline{A}_*$ and that $\operatorname{tr}_1(\overline{E}_*)_*|_{\widetilde{X}}$ are orthogonally split and corollary 3.8 we obtain

$$\begin{aligned} \mathrm{d}_{\mathcal{D}}\, T_C(\overline{\xi}) &= \sum_k (-1)^k \operatorname{ch}(\overline{E}_k) - \sum_k (-1)^k (p_P)_* \operatorname{ch}(K(\overline{F},\overline{N})_k) \\ &= \sum_k (-1)^k [\operatorname{ch}(\overline{E}_k)] - (p_P)_*[c_r(\overline{Q}) \operatorname{Td}^{-1}(\overline{Q})] \\ &= \sum_k (-1)^k [\operatorname{ch}(\overline{E}_k)] - i_*[\operatorname{ch}(\overline{F}) \operatorname{Td}^{-1}(\overline{N})]. \end{aligned}$$

We now prove the normalization property. We consider first the case when $Y = \emptyset$ and $\overline{E}_*$ is a non-negatively graded orthogonally split complex. We denote by

$$\overline{K}_i = \operatorname{Ker}(\mathrm{d}_i \colon E_i \longrightarrow E_{i-1})$$

with the induced metric. By hypothesis there are isometries

$$\overline{E}_i = \overline{K}_i \oplus \overline{K}_{i-1}.$$

Under these isometries, the differential is $\mathrm{d}(s,t) = (t,0)$. Following the explicit construction of $\operatorname{tr}_1(E_*)$ given in [20], recalled in definition 2.5, we see that

$$\operatorname{tr}_1(E_*)_i = p^* K_i \otimes q^* \mathcal{O}(i) \oplus p^* K_{i-1} \otimes q^* \mathcal{O}(i-1) = K_i(i) \oplus K_{i-1}(i-1).$$

Moreover, we can induce a metric on $\operatorname{tr}_1(E_*)_*$ satisfying the hypothesis of definition 2.9 by means of the metric of the bundles K_i and the Fubini-Study metric on the bundles $\mathcal{O}(i)$. It is clear that the second and third terms of the right hand side of equation (7.3) are zero. For the first term we have

$$\begin{aligned}\sum_k (-1)^k (p_W)_* W_1 \bullet \left(\operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_k)\right) \\ &= (p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\overline{K}_k(k) \overset{\perp}{\oplus} \overline{K}_{k-1}(k-1)) \right) \\ &= (p_W)_* \left(W_1 \bullet (a + b \wedge \omega) \right),\end{aligned}$$

where ω is the Fubini-Study $(1,1)$-form on $\mathbb{P}^1$ and a, b are inverse images of differential forms on X. Therefore we obtain that $T_C(\overline{E}_*) = 0$.
Now let $\overline{\xi} = (i \colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_*)$ and let $\overline{B}_*$ be a non-negatively graded orthogonally split complex of vector bundles. By [20] section 1.1, we have that $W(E_* \oplus B_*) = W(E_*)$ and that

$$\operatorname{tr}_1(E_* \oplus B_*) = \operatorname{tr}_1(E_*) \oplus \pi^* \operatorname{tr}_1(B_*).$$

In order to compute $T_C(\overline{\xi})$, we have to consider the exact sequences of hermitian vector bundles over P

$$\overline{\eta}_k \colon 0 \longrightarrow \overline{A}_k \longrightarrow \operatorname{tr}_1(\overline{E}_*)_k|_P \longrightarrow K(\overline{F}, \overline{N})_k \longrightarrow 0,$$

whereas, in order to compute $T_C(\overline{\xi} \oplus \overline{B}_*)$, we consider the sequences

$$\overline{\eta}'_k \colon$$
$$0 \longrightarrow \overline{A}_k \oplus \pi^*(\operatorname{tr}_1(\overline{B})_k)|_P \longrightarrow \operatorname{tr}_1(\overline{E}_*)_k \oplus \pi^*(\operatorname{tr}_1(\overline{B})_k)|_P \longrightarrow K(\overline{F}, \overline{N})_k \longrightarrow 0.$$

By the additivity of Bott-Chern classes, we have that $\widetilde{\mathrm{ch}}(\overline{\eta}_k)=\widetilde{\mathrm{ch}}(\overline{\eta}'_k)$. Therefore

$$\begin{aligned}T_C(\overline{\xi}\oplus\bar{B}_*)-T_C(\overline{\xi})&=-(p_W)_*\left(\sum_k(-1)^kW_1\bullet\mathrm{ch}(\mathrm{tr}_1(\overline{E}_*\oplus\overline{B}_*)_k)\right)\\&\qquad+(p_W)_*\left(\sum_k(-1)^kW_1\bullet\mathrm{ch}(\mathrm{tr}_1(\overline{E}_*)_k)\right)\\&=-(p_W)_*\left(\sum_k(-1)^kW_1\bullet\mathrm{ch}(\mathrm{tr}_1(\overline{B}_*)_k)\right)\\&=0.\end{aligned}$$

The proof of the functoriality is left to the reader.
Finally we prove that $C_{T_C}=C$. Let Y be a complex manifold and let $\overline{F}$ and $\overline{N}$ be two hermitian vector bundles. We write $X=\mathbb{P}(N\oplus\mathbb{C})$. Let $i\colon Y\longrightarrow X$ be the inclusion given by the zero section and let $\pi_X\colon X\longrightarrow Y$ be the projection. On X we have the tautological exact sequence

$$0\longrightarrow\mathcal{O}(-1)\longrightarrow\pi_X^*(N\oplus\mathbb{C})\longrightarrow Q\longrightarrow 0$$

and the Koszul resolution, denoted $K(\overline{F},\overline{N})$. We denote

$$\overline{\xi}=(i\colon Y\longrightarrow X,\overline{N},\overline{F},K(\overline{F},\overline{N})).$$

Using the definition of T_C, that is, equation (7.5), and the fact that T_C satisfies the properties of definition 6.9, hence equation (7.3) is satisfied, we obtain that

$$i_*C(F,N)=i_*C_{T_C}(F,N)$$

Applying $(\pi_X)_*$ we obtain that $C(F,N)=C_{T_C}(F,N)$ which finishes the proof of theorem 7.1. □

8 Transitivity and projection formula

We now investigate how different properties of the characteristic class C_T are reflected in the corresponding theory of singular Bott-Chern classes.

Proposition 8.1. *Let $i\colon Y\hookrightarrow X$ be a closed immersion of complex manifolds. Let $\overline{F}$ be a hermitian vector bundle on Y and $\overline{G}$ a hermitian vector bundle on X. Let $\overline{N}$ denote the normal bundle to Y provided with a hermitian metric. Let $\overline{E}_*$ be a finite resolution of i_*F by hermitian vector bundles. We denote $\overline{\xi}=(i\colon Y\longrightarrow X,\overline{N},\overline{F},\overline{E}_*)$ and $\overline{\xi}\otimes\overline{G}=(i\colon Y\longrightarrow X,\overline{N},\overline{F}\otimes i^*\overline{G},\overline{E}_*\otimes\overline{G})$. Then*

$$T(\overline{\xi}\otimes\overline{G})-T(\overline{\xi})\bullet\mathrm{ch}(\overline{G})=i_*(C_T(F\otimes i^*G,N))-i_*(C_T(F,N))\bullet\mathrm{ch}(\overline{G}).$$

Proof. Since the construction of $\operatorname{tr}_1(E_*)_*$ is local on X and Y and compatible with finite sums, we have that

$$W(E_*) = W(E_* \otimes G), \qquad \operatorname{tr}_1(\overline{E}_* \otimes \overline{G})_* = \operatorname{tr}_1(\overline{E}_*)_* \otimes p_W^* \overline{G}.$$

We first compute

$$\begin{aligned}(p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(\overline{E}_* \otimes \overline{G})_*) \right) \\ = (p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_*) p_W^* \operatorname{ch}(\overline{G}) \right) \\ = (p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(\overline{E}_*)_*) \right) \operatorname{ch}(\overline{G}). \quad (8.2)\end{aligned}$$

The Koszul resolution of $i_*(F \otimes i^*G)$ is given by

$$K(F \otimes i^*G, N) = K(F, N) \otimes p_P^* G.$$

For each $k \geq 0$, we will denote by $\overline{\eta}_k \otimes p_P^* \overline{G}$ the exact sequence

$$0 \longrightarrow \overline{A}_k \otimes p_P^* \overline{G} \longrightarrow \operatorname{tr}_1(\overline{E}_* \otimes \overline{G})_k|_P \longrightarrow K(\overline{F}, \overline{N})_k \otimes p_P^* \overline{G} \longrightarrow 0.$$

Then, we have

$$(p_P)_*[\widetilde{\operatorname{ch}}(\overline{\eta}_k \otimes p_P^* \overline{G})] = (p_P)_*[\widetilde{\operatorname{ch}}(\overline{\eta}_k) \bullet p_P^* \operatorname{ch}(\overline{G})] = (p_P)_*[\widetilde{\operatorname{ch}}(\overline{\eta}_k)] \bullet \operatorname{ch}(\overline{G}) \quad (8.3)$$

Thus the proposition follows from equation (8.2), equation (8.3) and formula (7.3). □

Definition 8.4. We will say that a theory of singular Bott-Chern classes is *compatible with the projection formula* if, whenever we are in the situation of proposition 8.1, the following equality holds:

$$T(\overline{\xi} \otimes \overline{G}) = T(\overline{\xi}) \bullet \operatorname{ch}(\overline{G}).$$

We will say that a characteristic class C (of pairs of vector bundles) is *compatible with the projection formula* if it satisfies

$$C(F, N) = C(\mathcal{O}_Y, N) \bullet \operatorname{ch}(F).$$

Corollary 8.5. *A theory of singular Bott-Chern classes T is compatible with the projection formula if and only if it is the case for the associated characteristic class C_T.*

Proof. Assume that C_T is compatible with the projection formula and that we are in the situation of proposition 8.1. Then

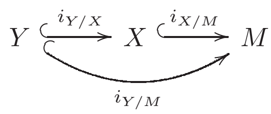
$$\begin{aligned} i_*C_T(F\otimes i^*G,N)) &= i_*(C_T(\mathcal{O}_Y,N)\bullet \operatorname{ch}(F\otimes i^*G)) \\ &= i_*(C_T(\mathcal{O}_Y,N)\bullet \operatorname{ch}(F) i^*\operatorname{ch}(G)) \\ &= i_*(C_T(\mathcal{O}_Y,N)\bullet \operatorname{ch}(F))\operatorname{ch}(G) \\ &= i_*(C_T(F,N))\bullet \operatorname{ch}(G). \end{aligned}$$

Thus, by proposition 8.1, T is compatible with the projection formula.
Assume that T is compatible with the projection formula. Let $\overline{F}$ and $\overline{N}$ be hermitian vector bundles over a complex manifold Y. Let $s\colon Y \hookrightarrow P := \mathbb{P}(N\oplus \mathbb{C})$ be the zero section and let $\pi\colon P \longrightarrow Y$ be the projection. Then

$$\begin{aligned} C_T(F,N) &= \pi_*(T(K(\overline{F},\overline{N}))) \\ &= \pi_*(T(K(\overline{\mathcal{O}}_Y,\overline{N})\otimes \pi^*\overline{F})) \\ &= \pi_*(T(K(\overline{\mathcal{O}}_Y,\overline{N}))\bullet \pi^*\operatorname{ch}(F)) \\ &= \pi_*(T(K(\overline{\mathcal{O}}_Y,\overline{N})))\bullet \operatorname{ch}(F) \\ &= C_T(\mathcal{O}_Y,N)\bullet \operatorname{ch}(F). \end{aligned}$$

□

We will next investigate the relationship between singular Bott-Chern classes and compositions of closed immersions. Thus, let



be a composition of closed immersions. Assume that the normal bundles $N_{Y/X}$, $N_{X/M}$ and $N_{Y/M}$ are provided with hermitian metrics. We will denote by $\overline{\varepsilon}$ the exact sequence

$$\overline{\varepsilon}\colon 0\to \overline{N}_{Y/X}\to \overline{N}_{Y/M}\to i^*_{Y/X}\overline{N}_{X/M}\to 0. \tag{8.6}$$

Let $P_{X/M}=\mathbb{P}(N_{X/M}\oplus\mathbb{C})$ be the projective completion of the normal cone to X in M. Then there is an isomorphism

$$N_{Y/P_{X/M}} \cong N_{Y/X}\oplus i^*_{Y/X}N_{X/M}. \tag{8.7}$$

We denote by $\overline{N}_{Y/P_{X/M}}$ the vector bundle on the left hand side with the hermitian metric induced by the isomorphism (8.7).
Let $\overline{F}$ be a hermitian vector bundle over Y, let $\overline{E}_*\longrightarrow (i_{Y/X})_*F$ be a resolution by hermitian vector bundles. Let $\overline{E}'_{*,*}$ be a complex of complexes of vector

bundles over M, such that, for each $k \geq 0$, $\overline{E}'_{k,*} \longrightarrow (i_{X/M})_* E_k$ is a resolution, and there is a commutative diagram of resolutions

$$\begin{array}{ccccccccc} \cdots & \longrightarrow & E'_{k+1,*} & \longrightarrow & E'_{k,*} & \longrightarrow & E'_{k-1,*} & \longrightarrow & \cdots . \\ & & \downarrow & & \downarrow & & \downarrow & & \\ \cdots & \longrightarrow & (i_{X/M})_* E_{k+1} & \longrightarrow & (i_{X/M})_* E_k & \longrightarrow & (i_{X/M})_* E_{k-1} & \longrightarrow & \cdots \end{array}$$

It follows that we have a resolution $\operatorname{Tot}(\overline{E}'_{*,*}) \longrightarrow (i_{Y/M})_* F$ of $(i_{Y/M})_* F$ by hermitian vector bundles.

Notation 8.8. We will denote

$$\begin{aligned} \overline{\xi}_{Y \hookrightarrow X} &= (i_{Y/X}, \overline{N}_{Y/X}, \overline{F}, \overline{E}_*), \\ \overline{\xi}_{Y \hookrightarrow M} &= (i_{Y/M}, \overline{N}_{Y/M}, \overline{F}, \operatorname{Tot}(\overline{E}'_{*,*})), \\ \overline{\xi}_{X \hookrightarrow M,k} &= (i_{X/M}, \overline{N}_{X/M}, \overline{E}_k, \overline{E}'_{k,*}). \end{aligned}$$

We will also denote by $\overline{\xi}_{Y \hookrightarrow P_{X/M}}$ the hermitian embedded vector bundle

$$\left(Y \hookrightarrow P_{X/M}, \overline{N}_{Y/P_{X/M}}, \overline{F}, \operatorname{Tot}(\pi^*_{P_{X/M}} \overline{E}_* \otimes K(\mathcal{O}_X, \overline{N}_{X/M})) \right).$$

Let T be a theory of singular Bott-Chern classes, and let C_T be its associated characteristic class. Our aim now is to relate $T(\overline{\xi}_{Y \hookrightarrow X})$, $T(\overline{\xi}_{Y \hookrightarrow M})$ and $T(\overline{\xi}_{X \hookrightarrow M,k})$.

Let W_X be the deformation to the normal cone of X in M. As before we denote by $j_X \colon X \times \mathbb{P}^1 \longrightarrow W_X$ the inclusion.

We denote by W the deformation to the normal cone of $j_X(Y \times \mathbb{P}^1)$ in W_X.

This double deformation is represented in figure 1. There is a proper map $q_W \colon W \longrightarrow \mathbb{P}^1 \times \mathbb{P}^1$. The fibers of q_W over the corners of $\mathbb{P}^1 \times \mathbb{P}^1$ are as follows:

$$\begin{aligned} q_W^{-1}(0,0) &= M, \\ q_W^{-1}(\infty,0) &= \widetilde{M}_X \times \{0\} \cup P_{X/M}, \\ q_W^{-1}(0,\infty) &= \widetilde{M}_Y \cup P_{Y/M}, \\ q_W^{-1}(\infty,\infty) &= \widetilde{M}_X \times \{\infty\} \cup \widetilde{P}_{X/M} \cup P_{Y/P_{X/M}}, \end{aligned}$$

where $\widetilde{M}_X$ and $\widetilde{M}_Y$ are the blow-up of M along X and Y respectively, $P_{Y/M} = \mathbb{P}(N_{Y/M} \oplus \mathbb{C})$ is the projective completion of the normal cone to Y in M, $P_{Y/P_{X/M}}$ of the normal cone to Y in $P_{X/M}$ and $\widetilde{P}_{X/M}$ is the blow-up of $P_{X/M}$

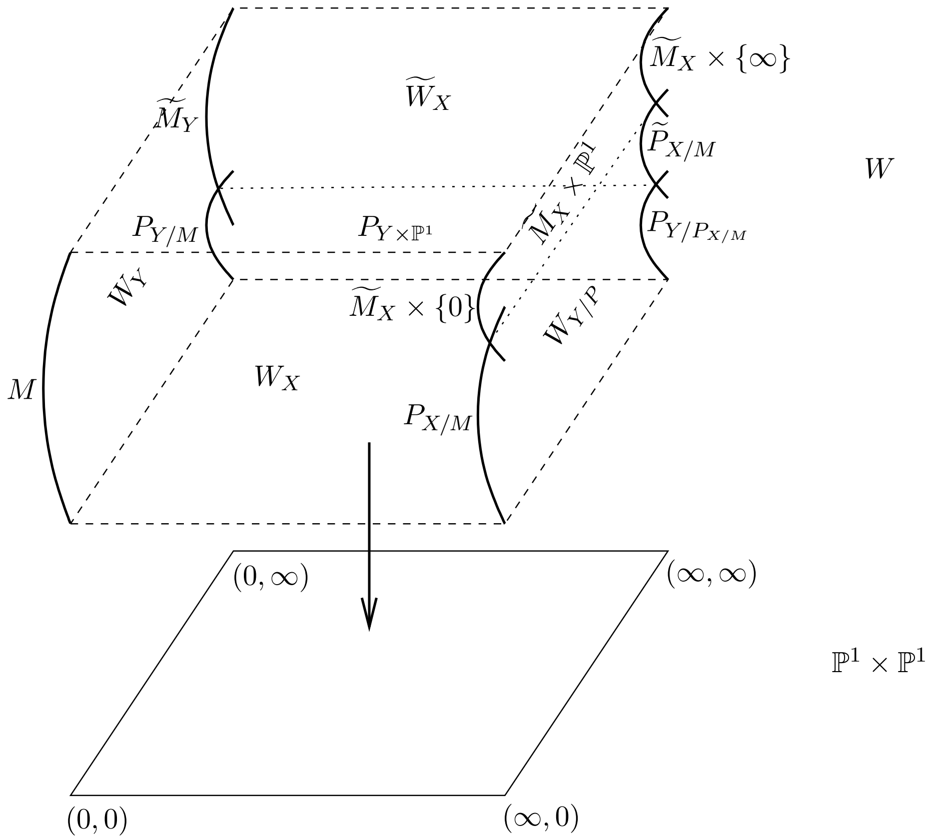


Figure 1: Double deformation

along Y. The preimages by π of the different faces of $\mathbb{P}^1 \times \mathbb{P}^1$ are as follows:

$$\begin{aligned} q_W^{-1}(\mathbb{P}^1 \times \{0\}) &= W_X, \\ q_W^{-1}(\{0\} \times \mathbb{P}^1) &= W_Y, \\ q_W^{-1}(\mathbb{P}^1 \times \{\infty\}) &= \widetilde{W}_X \cup P_{Y\times\mathbb{P}^1}, \\ q_W^{-1}(\{\infty\} \times \mathbb{P}^1) &= \widetilde{M}_X \times \mathbb{P}^1 \cup W_{Y/P}, \end{aligned}$$

where W_Y is the deformation to the normal cone of Y in M, the component $\widetilde{W}_X$ is the blow-up of W_X along $j_X(Y \times \mathbb{P}^1)$, while $P_{Y\times\mathbb{P}^1} = \mathbb{P}(N_{Y\times\mathbb{P}^1/W_X} \oplus \mathbb{C})$ is the projective completion of the normal cone to $j_X(Y \times \mathbb{P}^1)$ in W_X and $W_{Y/P}$ is the deformation to the normal cone of Y inside $P_{X/M}$. All the above subvarieties will be called boundary components of W.

We will use the following notations for the different maps.

$$
\begin{aligned}
&p_X\colon X\times\mathbb{P}^1\longrightarrow X && p_Y\colon Y\times\mathbb{P}^1\longrightarrow Y\\
&p_{Y\times\mathbb{P}^1}\colon Y\times\mathbb{P}^1\times\mathbb{P}^1\longrightarrow Y\times\mathbb{P}^1 && p_{\widetilde{M}_X\times\mathbb{P}^1}\colon \widetilde{M}_X\times\mathbb{P}^1\longrightarrow M\\
&p_{W_{Y/P}}\colon W_{Y/P}\longrightarrow M && p_{W_Y}\colon W_Y\longrightarrow M\\
&p_{W_X}\colon W_X\longrightarrow M && p_{P_{Y\times\mathbb{P}^1}}\colon P_{Y\times\mathbb{P}^1}\longrightarrow M\\
&p_{\widetilde{W}_X}\colon \widetilde{W}_X\longrightarrow M && p_{P_{Y/P_{X/M}}}\colon P_{Y/P_{X/M}}\longrightarrow M\\
&p_{P_{X/M}}\colon P_{X/M}\longrightarrow M && p_{\widetilde{P}_{X/M}}\colon \widetilde{P}_{X/M}\longrightarrow M\\
&p_{P_{Y/M}}\colon P_{Y/M}\longrightarrow M && p_W\colon W\longrightarrow M\\
&j_Y\colon Y\times\mathbb{P}^1\longrightarrow W_Y && j'_Y\colon Y\times\mathbb{P}^1\longrightarrow W_X\\
&j_{Y\times\mathbb{P}^1}\colon Y\times\mathbb{P}^1\times\mathbb{P}^1\longrightarrow W && i_{Y/P_{X/M}}\colon Y\longrightarrow P_{X/M}\\
&\pi_{P_{X/M}}\colon P_{X/M}\longrightarrow X && \pi_{P_{Y/M}}\colon P_{Y/M}\longrightarrow Y\\
&\pi_{P_{Y/P}}\colon P_{Y/P_{X/M}}\longrightarrow Y && \pi_{P_{Y\times\mathbb{P}^1}}\colon P_{Y\times\mathbb{P}^1}\longrightarrow Y\times\mathbb{P}^1\\
&\pi_{\widetilde{M}_X}\colon \widetilde{M}_X\longrightarrow M && \pi_{\widetilde{M}_Y}\colon \widetilde{M}_Y\longrightarrow M
\end{aligned}
$$

Note that the map $p_{\widetilde{M}_X\times\mathbb{P}^1}$ factors through the blow-up $\widetilde{M}_X\longrightarrow M$ and the map $p_{\widetilde{W}_X}$ factors through the blow-up $\widetilde{M}_Y\longrightarrow M$, whereas the maps $p_{W_{Y/P}}$, $p_{P_{X/M}}$ and $p_{\widetilde{P}_{X/M}}$ factor through the inclusion $X\hookrightarrow M$ and the maps $p_{P_{Y\times\mathbb{P}^1}}$, $p_{P_{Y/M}}$ and $p_{P_{Y/P_{X/M}}}$ factor through the inclusion $Y\hookrightarrow M$.
The normal bundle to $X\times\mathbb{P}^1$ in W_X is isomorphic to $p_X^*N_{X/M}\otimes q_X^*\mathcal{O}(-1)$ and we consider on it the metric induced by the metric on $\overline{N}_{X/M}$ and the Fubini-Study metric on $\mathcal{O}(-1)$. We denote it by $\overline{N}_{X\times\mathbb{P}^1/W_X}$. The normal bundle to $Y\times\mathbb{P}^1$ in W_X satisfies

$$
\begin{aligned}
N_{Y\times\mathbb{P}^1/W_X}|_{Y\times\{0\}}&\cong N_{Y/M}\\
N_{Y\times\mathbb{P}^1/W_X}|_{Y\times\{\infty\}}&\cong N_{Y/X}\oplus i_{Y/X}^*N_{X/M}.
\end{aligned}
$$

On $N_{Y\times\mathbb{P}^1/W_X}$ we choose a hermitian metric such that the above isomorphisms are isometries. Finally, on the normal bundle to $Y\times\mathbb{P}^1\times\mathbb{P}^1$ in W, we define a metric using the same procedure as the definition of the metric of $\overline{N}_{X\times\mathbb{P}^1/W_X}$.
On W_X we obtain a sequence of resolutions $\operatorname{tr}_1(\overline{E}')_{n,*}\longrightarrow(j_X)_*p_X^*E_n$. They form a complex of complexes $\operatorname{tr}_1(\overline{E}')_{*,*}$ and the associated total complex $\operatorname{Tot}(\operatorname{tr}_1(\overline{E}')_{*,*})$ provides us with a resolution

$$\operatorname{Tot}(\operatorname{tr}_1(\overline{E}')_{*,*})_*\longrightarrow(j'_Y)_*p_Y^*F. \tag{8.9}$$

The restriction of $\operatorname{Tot}(\operatorname{tr}_1(\overline{E}')_{*,*})$ to M is $\operatorname{Tot}(\overline{E}'_{*,*})$. The restriction of each complex $\operatorname{tr}_1(\overline{E}')_{n,*}$ to $\widetilde{M}_X\times\{0\}$ is orthogonally split. Therefore the restriction of $\operatorname{Tot}(\operatorname{tr}_1(\overline{E}'))$ to $\widetilde{M}_X\times\{0\}$ is the total complex of a complex of orthogonally split complexes. So it is acyclic although not necessarily orthogonally split. The restriction of each complex $\mathrm{tr}_1(\overline{E}')_{n,*}$ to $P_{X/M}$ fits in an exact sequence

$$0 \longrightarrow \overline{A}_{n,*} \longrightarrow \mathrm{tr}_1(\overline{E}')_{n,*}|_{P_{X/M}} \longrightarrow \pi^*_{P_{X/M}}\overline{E}_n \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_* \longrightarrow 0.$$

These exact sequences glue together giving a commutative diagram

$$\begin{array}{ccccc} \mathrm{Tot}(\overline{A}_{*,*}) & \hookrightarrow & \mathrm{Tot}(\mathrm{tr}_1(\overline{E}')_{*,*}|_{P_{X/M}}) & \twoheadrightarrow & \mathrm{Tot}(\pi^*_{P_{X/M}}\overline{E}_* \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_*) \\ \downarrow & & \downarrow & & \downarrow \\ 0 & \hookrightarrow & (i_{Y/P_{X/M}})_*F & \twoheadrightarrow & (i_{Y/P_{X/M}})_*F \end{array}$$

where the rows are short exact sequences. Even if the complexes $(\overline{A}_n)_*$ are orthogonally split, this is not necessarily the case for $\mathrm{Tot}(\overline{A}_{*,*})$. To ease the notation we will denote $\overline{A}_* = \mathrm{Tot}(\overline{A}_{*,*})$.

Applying theorem 5.4 to the resolution (8.9), we obtain a complex of hermitian vector bundles $\widetilde{E}'_* = \mathrm{tr}_1(\mathrm{Tot}(\mathrm{tr}_1(\overline{E}')_{*,*}))$ which is a resolution of the coherent sheaf $(j_{Y\times\mathbb{P}^1})_*p^*_{Y\times\mathbb{P}^1}p^*_Y F$.

We now study the restriction of $\widetilde{E}'_*$ to each of the boundary components of W.

- The restriction of $\widetilde{E}'_*$ to W_X is just $\mathrm{Tot}(\mathrm{tr}_1(\overline{E}'))$ which has already been described. For each $k \geq 0$, we will denote by η^1_k the short exact sequence of hermitian vector bundles on $P_{X/M}$

  $$\overline{A}_k \hookrightarrow \mathrm{Tot}(\mathrm{tr}_1(\overline{E}')_{*,*}|_{P_{X/M}})_k \twoheadrightarrow \mathrm{Tot}(\pi^*_{P_{X/M}}\overline{E} \otimes K(\mathcal{O}_X, \overline{N}_{X/M}))_k\ ,$$

  whereas, for each $n, k \geq 0$ we will denote by $\eta^1_{n,k}$ the short exact sequence

  $$\overline{A}_{n,k} \hookrightarrow \mathrm{tr}_1(\overline{E}')_{n,k}|_{P_{X/M}} \twoheadrightarrow \pi^*_{P_{X/M}}\overline{E}_n \otimes K(\mathcal{O}_X, \overline{N}_{X/M})_k\ .$$

- Its restriction to W_Y is $\mathrm{tr}_1(\mathrm{Tot}(\overline{E}'))$. It is a resolution of $(j_Y)_*p^*_Y F$. Its restriction to $\widetilde{M}_Y$ is orthogonally split, whereas its restriction to $P_{Y/M}$ fits in an exact sequence

  $$0 \longrightarrow \overline{B}_* \longrightarrow \mathrm{tr}_1(\mathrm{Tot}(\overline{E}'))_*|_{P_{Y/M}} \longrightarrow \pi^*_{P_{Y/M}}\overline{F} \otimes K(\overline{\mathcal{O}}_Y, \overline{N}_{Y/M}) \longrightarrow 0.$$

  For each $k \geq 0$ we will denote by η^2_k the degree k piece of the above exact sequence.

- Its restriction to $\widetilde{M}_X \times \mathbb{P}^1$ is an acyclic complex, such that its further restriction to $\widetilde{M}_X \times \{0\}$ is acyclic and its restriction to $\widetilde{M}_X \times \{\infty\}$ is orthogonally split.

- Its restriction to $W_{Y/P}$ fits in a short exact sequence

$$0 \to \mathrm{tr}_1(\overline{A}_*) \to \widetilde{E}'_*|_{W_{Y/P}} \to \mathrm{tr}_1(\mathrm{Tot}(\pi^*_{P_{X/M}}\overline{E} \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M}))) \to 0.$$

For each $k \geq 0$, we will denote by μ^1_k the exact sequence of hermitian vector bundles over $W_{Y/P}$ given by the piece of degree k of this exact sequence. The three terms of the above exact sequence become orthogonally split when restricted to $\widetilde{P}_{X/M}$. By contrast, when restricted to $P_{Y/P_{X/M}}$ they fit in a commutative diagram

$$\begin{array}{ccccc}
\overline{C}^1_* & \hookrightarrow & \overline{C}^2_* & \twoheadrightarrow & \overline{C}^3 \\
\downarrow & & \downarrow & & \downarrow \\
\mathrm{tr}_1(\overline{A})_*|_{P_{Y/P_{X/M}}} & \hookrightarrow & \widetilde{E}'_*|_{P_{Y/P_{X/M}}} & \twoheadrightarrow & \overline{D}^2_* \\
\downarrow & & \downarrow & & \downarrow \\
0 & \hookrightarrow & \overline{D}^1_* & \twoheadrightarrow & \overline{D}^1_*
\end{array}$$

where the complexes $\overline{C}^i_*$ are orthogonally split, and

$$\overline{D}^1_* = \pi^*_{P_{Y/P}}\overline{F} \otimes K(\overline{\mathcal{O}}_Y, \overline{N}_{Y/P_{X/M}}),$$
$$\overline{D}^2_* = \mathrm{tr}_1(\mathrm{Tot}(\pi^*_{P_{X/M}}\overline{E} \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})))|_{P_{Y/P_{X/M}}}.$$

For each $k \geq 0$, we will denote by η^3_k the exact sequence corresponding to the piece of degree k of the second row of the above diagram, by η^4_k that of the second column and by η^5_k that of the third column. Notice that the map in the third row is an isometry. We assume that the metric on C^1_* is chosen in such a way that the first column is an isometry. Since the complexes $\overline{C}^i_*$ are orthogonally split, by lemma 2.17 we obtain

$$\sum_k (-1)^k \left(\widetilde{\mathrm{ch}}(\eta^3_k) - \widetilde{\mathrm{ch}}(\eta^4_k) + \widetilde{\mathrm{ch}}(\eta^5_k) \right) = 0. \qquad (8.10)$$

Note that the restriction of μ^1_k to $P_{X/M}$ agrees with η^1_k, whereas its restriction to $P_{Y/P_{X/M}}$ agrees with η^3_k.

- Its restriction to $\widetilde{W}_X$ is orthogonally split.

- Finally its restriction to $P_{Y\times\mathbb{P}^1}$ fits in an exact sequence

$$\overline{D}_* \hookrightarrow \widetilde{E}'_*|_{P_{Y\times\mathbb{P}^1}} \twoheadrightarrow \pi^*_{P_{Y\times\mathbb{P}^1}} p^*_{Y\times\mathbb{P}^1}\overline{F} \otimes K(\mathcal{O}_{Y\times\mathbb{P}^1}, \overline{N}_{Y\times\mathbb{P}^1/W_X}),$$

where $\overline{D}_*$ is orthogonally split. For each $k \geq 0$ we will denote by μ_k^2 the piece of degree k of this exact sequence. Note that the restriction of μ_k^2 to $P_{Y/M}$ agrees with η_k^2 and the restriction of μ_k^2 to $P_{Y/P_{X/M}}$ agrees with η_k^4.

On $\mathbb{P}^1 \times \mathbb{P}^1$ we denote the two projections by p_1 and p_2. Since the currents $p_1^* W_1$ and $p_2^* W_1$ have disjoint wave front sets we can define the current $W_2 = p_1^* W_1 \bullet p_2^* W_1 \in \mathcal{D}_D^2(\mathbb{P}^1 \times \mathbb{P}^1, 2)$ which satisfies

$$\mathrm{d}_{\mathcal{D}} W_2 = (\delta_{\{\infty\}\times\mathbb{P}^1} - \delta_{\{0\}\times\mathbb{P}^1}) \bullet p_2^* W_1 - p_1^* W_1 \bullet (\delta_{\mathbb{P}^1\times\{\infty\}} - \delta_{\mathbb{P}^1\times\{0\}}). \quad (8.11)$$

The key point in order to study the compatibility of singular Bott-Chern classes and composition of closed immersions is that, in the group $\bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(M,p)$, we have

$$\mathrm{d}_{\mathcal{D}}(p_W)_* \left(\sum_k (-1)^k W_2 \bullet \mathrm{ch}(\widetilde{E}'_k) \right) = 0.$$

We compute this class using the equation (8.11). It can be decomposed as follows.

$$\begin{aligned}
\mathrm{d}_{\mathcal{D}}(p_W)_* \left(\sum_k (-1)^k W_2 \bullet \mathrm{ch}(\widetilde{E}'_k) \right) = \\
(p_{\widetilde{M}_X\times\mathbb{P}^1})_* \left(\sum_k (-1)^k W_1 \bullet \mathrm{ch}(\widetilde{E}'_k|_{\widetilde{M}_X\times\mathbb{P}^1}) \right) && \text{(a)}\\
+ (p_{W_{Y/P}})_* \left(\sum_k (-1)^k W_1 \bullet \mathrm{ch}(\widetilde{E}'_k|_{W_{Y/P}}) \right) && \text{(b)}\\
- (p_{W_Y})_* \left(\sum_k (-1)^k W_1 \bullet \mathrm{ch}(\widetilde{E}'_k|_{W_Y}) \right) && \text{(c)}\\
- (p_{\widetilde{W}_X})_* \left(\sum_k (-1)^k W_1 \bullet \mathrm{ch}(\widetilde{E}'_k|_{\widetilde{W}_X}) \right) && \text{(d)}\\
- (p_{P_{Y\times\mathbb{P}^1}})_* \left(\sum_k (-1)^k W_1 \bullet \mathrm{ch}(\widetilde{E}'_k|_{P_{Y\times\mathbb{P}^1}}) \right) && \text{(e)}\\
+ (p_{W_X})_* \left(\sum_k (-1)^k W_1 \bullet \mathrm{ch}(\widetilde{E}'_k|_{W_X}) \right) && \text{(f)}\\
=: I_a + I_b - I_c - I_d - I_e + I_f
\end{aligned}$$

We compute each of the above terms.
(a) Since the restriction $\widetilde{E}'|_{\widetilde{M}_X\times\{\infty\}}$ is orthogonally split, we have

$$I_a = -(\pi_{\widetilde{M}_X})_* \widetilde{\mathrm{ch}}(\widetilde{E}'|_{\widetilde{M}_X\times\{0\}}).$$

But, using lemma 2.17 and the fact, for each k, the complexes $\operatorname{tr}_1(\overline{E}')_{k,*}|_{\widetilde{M}_X}$ are orthogonally split, we obtain that $I_a = 0$.
(b) We compute

$$\begin{aligned}
I_b =&(p_{W_{Y/P}})_*\left(\sum_k(-1)^k W_1 \bullet \operatorname{ch}(\widetilde{E}'_k|_{W_{Y/P}})\right)\\
=&(p_{W_{Y/P}})_*\Bigg(W_1 \bullet \sum_k(-1)^k(-\operatorname{d}_{\mathcal{D}}\widetilde{\operatorname{ch}}(\mu_k^1) + \operatorname{ch}(\operatorname{tr}_1(\overline{A}_*)_k)\\
&\qquad + \operatorname{ch}(\operatorname{tr}_1(\operatorname{Tot}(\pi^*_{P_{X/M}}\overline{E}\otimes K(\mathcal{O}_X,\overline{N}_{X/M})))_k))\Bigg)\\
=&\sum_k(-1)^k(-(p_{P_{Y/P_{X/M}}})_*\widetilde{\operatorname{ch}}(\eta_k^3) - (p_{\widetilde{P}_{X/M}})_*\widetilde{\operatorname{ch}}(\mu_k^1|_{\widetilde{P}_{X/M}}) + (p_{P_{X/M}})_*\widetilde{\operatorname{ch}}(\eta_k^1))\\
&- \widetilde{\operatorname{ch}}(\overline{A})\\
&- (i_{X/M})_*(\pi_{P_{X/M}})_*T(\overline{\xi}_{Y\hookrightarrow P_{X/M}}) + (i_{Y/M})_*C_T(F,N_{Y/P_{X/M}})\\
&- \sum_k(-1)^k(p_{P_{Y/P_{X/M}}})\widetilde{\operatorname{ch}}(\eta_k^5),
\end{aligned}$$

where $\xi_{Y\hookrightarrow P_{X/M}}$ is as in notation 8.8.
By corollary 2.19 and the fact that the exact sequences $\overline{A}_{k,*}$ are orthogonally split, the term $\widetilde{\operatorname{ch}}(\overline{A})$ vanishes.
Also by corollary 2.19 we can see that

$$\sum_k(-1)^k(p_{\widetilde{P}_{X/M}})_*\widetilde{\operatorname{ch}}(\mu_k^1|_{\widetilde{P}_{X/M}})$$

vanishes.
Therefore we conclude

$$\begin{aligned}
I_b =&\sum_k(-1)^k(-(p_{P_{Y/P_{X/M}}})_*\widetilde{\operatorname{ch}}(\eta_k^3) + (p_{P_{X/M}})_*\widetilde{\operatorname{ch}}(\eta_k^1)) - (p_{P_{Y/P_{X/M}}})\widetilde{\operatorname{ch}}(\eta_k^5)\\
&- (i_{X/M})_*(\pi_{P_{X/M}})_*T(\overline{\xi}_{Y\hookrightarrow P_{X/M}}) + (i_{Y/M})_*C_T(F,N_{Y/P_{X/M}}).
\end{aligned}$$

(c) By the definition of singular Bott-Chern forms we have

$$I_c = -T(\overline{\xi}_{Y\hookrightarrow M}) + (i_{Y/M})_*C_T(F,N_{Y/M}) - \sum_k(-1)^k(p_{P_{Y/M}})_*\widetilde{\operatorname{ch}}(\eta_k^2),$$

(d) Since the restriction of $\widetilde{E}'_*$ to $\widetilde{W}_X$ is orthogonally split, we have $I_d = 0$.

(e) We compute

$$\begin{aligned}I_e =&(p_{P_{Y\times\mathbb{P}^1}})_*\left(\sum_k(-1)^k W_1\bullet \mathrm{ch}(\widetilde{E}'_k|_{P_{Y\times\mathbb{P}^1}})\right)\\ =&(p_{P_{Y\times\mathbb{P}^1}})_*\Bigg(W_1\bullet\sum_k(-1)^k\big(-\mathrm{d}_{\mathcal{D}}\,\widetilde{ch}(\mu_k^2)+\mathrm{ch}(\overline{D}_k)\\ &\qquad +\mathrm{ch}(\pi^*_{P_{Y\times\mathbb{P}^1}}p_Y^*\overline{F}\otimes K(\mathcal{O}_{Y\times\mathbb{P}^1},\overline{N}_{Y\times\mathbb{P}^1/W_X})_k)\big)\Bigg).\end{aligned}$$

The term $\sum(-1)^k\,\mathrm{ch}(\overline{D}_k)$ vanishes because the complex D_* is orthogonally split. We have

$$\begin{aligned}&\sum_k(-1)^k(p_{P_{Y\times\mathbb{P}^1}})_*(W_1\bullet\mathrm{ch}(\pi^*_{P_{Y\times\mathbb{P}^1}}p_Y^*\overline{F}\otimes K(\overline{\mathcal{O}}_{Y\times\mathbb{P}^1},\overline{N}_{Y\times\mathbb{P}^1/W_X})_k))\\ &=(i_{Y/M})_*\,\mathrm{ch}(\overline{F})\bullet(p_Y)_*\left(W_1\bullet\pi^*_{P_{Y\times\mathbb{P}^1}}\sum_k(-1)^k\,\mathrm{ch}(K(\overline{\mathcal{O}}_{Y\times\mathbb{P}^1},\overline{N}_{Y\times\mathbb{P}^1/W_X})_k)\right)\\ &\qquad=(i_{Y/M})_*\,\mathrm{ch}(\overline{F})\bullet(p_Y)_*\left(W_1\bullet\mathrm{Td}^{-1}(\overline{N}_{Y\times\mathbb{P}^1/W_X})\right)\\ &\qquad\qquad=(i_{Y/M})_*\,\mathrm{ch}(\overline{F})\bullet\widetilde{\mathrm{Td}^{-1}}(\overline{\varepsilon}_N),\end{aligned}\tag{8.12}$$

where $\overline{\varepsilon}_N$ is the exact sequence (8.6).
Therefore we obtain

$$\begin{aligned}I_e=&-\sum_k(-1)^k(p_{P_{Y/P_{X/M}}})_*\widetilde{\mathrm{ch}}(\eta_k^4)+\sum_k(-1)^k(p_{P_{Y/M}})_*\widetilde{\mathrm{ch}}(\eta_k^2)\\ &+(i_{Y/M})_*\,\mathrm{ch}(\overline{F})\bullet\widetilde{\mathrm{Td}^{-1}}(\overline{\varepsilon}_N).\end{aligned}$$

(f) Finally we have

$$\begin{aligned}I_f=&-\sum_k(-1)^kT(\overline{\xi}_{X\hookrightarrow M,k})+\sum_k(-1)^k(i_{X/M})_*C_T(E_k,N_{X/M})\\ &-\sum_{k,l}(-1)^{k+l}(p_{P_{X/M}})_*\widetilde{\mathrm{ch}}(\eta^1_{k,l}).\end{aligned}$$

By corollary 2.19 we have that

$$\sum_{m,l}(-1)^{m+l}(p_{P_{X/M}})_*\widetilde{\mathrm{ch}}(\eta^1_{m,l})=\sum_k(-1)^k(p_{P_{X/M}})_*\widetilde{\mathrm{ch}}(\eta^1_k).$$

Thus

$$\begin{aligned}I_f=&-\sum_k(-1)^kT(\overline{\xi}_{X\hookrightarrow M,k})+\sum_k(-1)^k(i_{X/M})_*C_T(E_k,N_{X/M})\\ &-\sum_k(-1)^k(p_{P_{X/M}})_*\widetilde{\mathrm{ch}}(\eta^1_k).\end{aligned}$$

Summing up all the terms we have computed, and taking into account equation (8.10) and the fact that

$$C_T(F, N_{Y/M}) = C_T(F, N_{Y/P_{X/M}})$$

we have obtained the following partial result.

Lemma 8.13. *Let $i_{Y/M} = i_{X/M} \circ i_{Y/X}$ be a composition of closed immersions of complex manifolds. Let T be a theory of singular Bott-Chern classes with C_T its associated characteristic class. Let $\overline{\xi}_{Y\hookrightarrow M}$, $\overline{\xi}_{X\hookrightarrow M,k}$ and $\overline{\xi}_{Y\hookrightarrow P_{X/M}}$ be as in notation 8.8, and let $\overline{\varepsilon}$ be as in* (8.6)*. Then, in the group $\bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(M,p)$, the equation*

$$\begin{aligned} T(\overline{\xi}_{Y\hookrightarrow M}) = \sum_k (-1)^k T(\overline{\xi}_{X\hookrightarrow M,k}) - \sum_k (-1)^k (i_{X/M})_* C_T(E_k, N_{X/M}) \\ + (i_{X/M})_*(\pi_{P_{X/M}})_* T(\overline{\xi}_{Y\hookrightarrow P_{X/M}}) + (i_{Y/M})_* \operatorname{ch}(\overline{F}) \bullet \widetilde{\operatorname{Td}^{-1}}(\overline{\varepsilon}_N) \end{aligned} \quad (8.14)$$

holds.

In order to compute the third term of the right hand side of equation (8.14) we consider the following situation

$$\begin{array}{ccc} Y \times_X P_{X/M} & \xrightarrow{\ j\ } & P_{X/M} \\ \pi \downarrow \uparrow s & & \pi \downarrow \uparrow s \\ Y & \xrightarrow{\ i\ } & X \end{array}.$$

To ease the notation, we denote $P_{X/M}$ by P, $Y \underset{X}{\times} P_{X/M}$ by X' and we denote by P' the projective completion of the normal cone to X' in P and by $\pi_{P'}\colon P' \longrightarrow X'$, $\pi_{X'/Y}\colon X' \longrightarrow Y$ and $\pi_{P'/Y}\colon P' \longrightarrow Y$ the projections. Observe that X and X' intersect transversely along Y. Moreover, $N_{Y/X'} = i^*_{Y/X} N_{X/M}$, $N_{X'/P} = \pi^*_{X'/Y} N_{Y/X}$ and $N_{Y/P} = N_{Y/X} \oplus N_{Y/X'}$. We use these identifications to define metrics on $N_{Y/X'}$, $N_{X'/P}$ and $N_{Y/P}$. Therefore the exact sequence

$$0 \longrightarrow \overline{N}_{Y/X'} \longrightarrow \overline{N}_{Y/P} \longrightarrow i^*_{Y/X'} \overline{N}_{X'/P} \longrightarrow 0$$

is orthogonally split.
We apply the previous lemma to the composition of closed inclusions

$$Y \hookrightarrow X' \hookrightarrow P,$$

the vector bundle $\overline{F}$ over Y and the resolutions

$$\begin{gathered} \pi^*\overline{F} \otimes j^* K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_* \longrightarrow s_* F \\ \pi^*\overline{E}_* \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_k \longrightarrow j_*(\pi^* F \otimes j^* K(\mathcal{O}_X, N_{X/M})_k). \end{gathered}$$

We denote by $\overline{\xi}_{Y\hookrightarrow P}$ and $\overline{\xi}_{X'\hookrightarrow P,k}$ the hermitian embedded vector bundles corresponding to the above resolutions. If $i_{Y/P'}: Y \hookrightarrow P'$ is the induced inclusion, we denote by $\overline{\xi}_{Y\hookrightarrow P'}$ the hermitian embedded vector bundle

$$\left(i_{Y/P'}, \overline{N}_{Y/P'}, \overline{F}, \operatorname{Tot}(\pi^*_{P'} j^* K(\overline{\mathcal{O}}_X, \overline{N}_{X/M}) \otimes K(\overline{\mathcal{O}}_{X'}, \overline{N}_{X'/P}) \otimes (\pi_{P'/Y})^* \overline{F})\right).$$

Note that the hermitian embedded vector bundle $\overline{\xi}_{Y\hookrightarrow P}$ agrees with the hermitian embedded vector bundle denoted $\overline{\xi}_{Y\hookrightarrow P_{X/M}}$ in lemma 8.13. Moreover, we have that

$$\overline{\xi}_{X'\hookrightarrow P,k} = \pi^* \overline{\xi}_{Y\hookrightarrow X} \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_k.$$

Applying lemma 8.13, we obtain

$$\begin{aligned} T(\overline{\xi}_{Y\hookrightarrow P_{X/M}}) = {} & \sum_k (-1)^k T(\overline{\xi}_{X'\hookrightarrow P_{X/M},k}) \\ & - \sum_k (-1)^k j_* C_T(\pi^* F \otimes j^* K(\mathcal{O}_X, N_{X/M})_k, N_{X'/P}) \\ & + j_*(\pi_{P'})_* T(\overline{\xi}_{Y\hookrightarrow P'}) \qquad (8.15) \end{aligned}$$

By proposition 8.1,

$$\begin{aligned} \sum_k (-1)^k T(\overline{\xi}_{X'\hookrightarrow P_{X/M},k}) &= \sum_k (-1)^k T(\pi^* \overline{\xi}_{Y\hookrightarrow X} \otimes K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_k) \\ &= T(\pi^* \overline{\xi}_{Y\hookrightarrow X}) \bullet \sum_k (-1)^k \operatorname{ch}(K(\overline{\mathcal{O}}_X, \overline{N}_{X/M})_k) \\ &\quad + \sum_k (-1)^k j_* C_T(\pi^* F \otimes j^* K(\mathcal{O}_X, N_{X/M})_k, N_{X'/P}) \\ &\quad - \sum_k (-1)^k j_* C_T(\pi^* F, N_{X'/P}) \bullet \operatorname{ch}(K(\mathcal{O}_X, N_{X/M})_k) \qquad (8.16) \end{aligned}$$

We now want to compute the term $(i_{X/M})_*(\pi_{P_{X/M}})_* j_*(\pi_{P'})_* T(\overline{\xi}_{Y\hookrightarrow P'})$. Observe that we can identify

$$P' = \mathbb{P}(i^*_{Y/X} N_{X/M} \oplus \mathbb{C}) \underset{Y}{\times} \mathbb{P}(s^* N_{X'/P} \oplus \mathbb{C}),$$

where $s^* N_{X'/P}$ is canonically isomorphic to $N_{Y/X}$.
Moreover

$$(i_{X/M})_*(\pi_{P_{X/M}})_* j_*(\pi_{P'})_* T(\overline{\xi}_{Y\hookrightarrow P'}) = (i_{Y/M})_*(\pi_{P'/Y})_* T(\overline{\xi}_{Y\hookrightarrow P'}).$$

Definition 8.17. We denote

$$C_T^{\mathrm{ad}}(F, N_{Y/X}, i^*_{Y/X} N_{X/M}) = (\pi_{P'/Y})_* T(\overline{\xi}_{Y\hookrightarrow P'})$$

and we define

$$\rho(F, N_{Y/X}, i^*_{Y/X} N_{X/M}) = C_T(F, N_{Y/M}) - C_T^{\mathrm{ad}}(F, N_{Y/X}, i^*_{Y/X} N_{X/M}). \quad (8.18)$$

Lemma 8.19. *The current* $C_T^{\mathrm{ad}}(F, N_{Y/X}, i^*_{Y/X}N_{X/M})$ *is closed and defines a characteristic class of triples of vector bundles. Therefore* ρ *is also a characteristic class. Moreover the class* ρ *does not depend on the theory of singular Bott-Chern classes* T.

Proof. The fact that $C_T^{\mathrm{ad}}(F, N_{Y/X}, i^*_{Y/X}N_{X/M})$ is closed and determines a characteristic class is proved as in 6.16. The independence of ρ from to T is seen as follows. We denote by $\overline{K}'_*$ the complex

$$\mathrm{Tot}(\pi^*_{P'}j^*K(\overline{\mathcal{O}}_X, \overline{N}_{X/M}) \otimes K(\overline{\mathcal{O}}_{X'}, \overline{N}_{X'/P})) \otimes (\pi_{P'/Y})^*\overline{F}.$$

This complex is a resolution of $(i_{Y/P'})_*\overline{F}$
Let W be the blow-up of $P' \times \mathbb{P}^1$ along $Y \times \infty$, and let $\mathrm{tr}_1(\overline{K}')_*$ be the deformation of complexes on W given by theorem 5.4. Just by looking at the rank of the different vector bundles we see that the restriction of $\mathrm{tr}_1(\overline{K}')_*$ to $P_{Y/P'}$, the exceptional divisor of this blow-up, is isomorphic (although not necessarily isometric) to the Koszul complex $K(\overline{F}, \overline{N}_{X/M})_*$. Then, by equation (7.3)

$$\begin{aligned} T(\overline{\xi}_{Y\hookrightarrow P'}) - (i_{Y/P'})_*C_T(F, N_{Y/M}) = \\ & - (p_W)_*\left(W_1 \bullet \sum_k (-1)^k \,\mathrm{ch}(\mathrm{tr}_1(\overline{K}')_k)\right) \\ & - \sum_k (-1)^k (p_P)_*\widetilde{\mathrm{ch}}(\mathrm{tr}_1(\overline{K}')_k|_{P_{Y/P'}}, K(\overline{F}, \overline{N}_{X/M})_k). \end{aligned}$$

Since the right hand side of this equation does not depend on the theory T, the result is proved. ☐

Using equations (8.15), (8.16), lemma 8.19 and the projection formula, we obtain

$$\begin{aligned} (\pi_{P_{X/M}})_*T(\overline{\xi}_{Y\hookrightarrow P_{X/M}}) &= \big(T(\overline{\xi}_{Y\hookrightarrow X}) - (i_{Y/X})_*C_T(F, N_{Y/X})\big) \\ &\qquad \bullet (\pi_{P_{X/M}})_* \sum_k (-1)^k \,\mathrm{ch}(K(\mathcal{O}_X, \overline{N}_{X/M})_k) \\ &\quad + (\pi_{P_{X/M}})_* j_*(\pi_{P'})_*T(\overline{\xi}_{Y\hookrightarrow P'}) \\ &= \big(T(\overline{\xi}_{Y\hookrightarrow X}) - (i_{Y/X})_*C_T(F, N_{Y/X})\big) \bullet \mathrm{Td}^{-1}(\overline{N}_{X/M}) \\ &\quad + (i_{Y/X})_*C_T^{\mathrm{ad}}(F, N_{Y/X}, i^*_{Y/X}N_{X/M}) \\ &= \big(T(\overline{\xi}_{Y\hookrightarrow X}) - (i_{Y/X})_*C_T(F, N_{Y/X})\big) \bullet \mathrm{Td}^{-1}(\overline{N}_{X/M}) \\ &\quad + (i_{Y/X})_*C_T(F, N_{Y/M}) - \rho(F, N_{Y/X}, i^*_{Y/X}N_{X/M}). \end{aligned} \tag{8.20}$$

Joining this equation and lemma 8.13 we obtain the main relationship between singular Bott-Chern classes and composition of closed immersions.

Proposition 8.21. *Let $i_{Y/M} = i_{X/M} \circ i_{Y/X}$ be a composition of closed immersions of complex manifolds. Let T be a theory of singular Bott-Chern classes with C_T its associated characteristic class. Let $\overline{\xi}_{Y\hookrightarrow M}$, $\overline{\xi}_{X\hookrightarrow M,k}$ and $\overline{\xi}_{Y\hookrightarrow P_{X/M}}$ be as in notation 8.8 and let $\overline{\varepsilon}$ be as in* (8.6). *Then, in the group $\bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(M,p)$, we have the equation*

$$\begin{aligned}T(\overline{\xi}_{Y\hookrightarrow M}) = \sum_k (-1)^k T(\overline{\xi}_{X\hookrightarrow M,k}) + (i_{X/M})_*(T(\overline{\xi}_{Y\hookrightarrow X}) \bullet \operatorname{Td}^{-1}(\overline{N}_{X/M}))\\ + (i_{Y/M})_* \operatorname{ch}(\overline{F}) \bullet \widetilde{\operatorname{Td}^{-1}}(\overline{\varepsilon}_N)\\ + (i_{Y/M})_* C_T^{\mathrm{ad}}(F, N_{Y/X}, i_{Y/X}^* N_{X/M})\\ - (i_{X/M})_*((i_{Y/X})_* C_T(F, N_{Y/X}) \bullet \operatorname{Td}^{-1}(N_{X/M}))\\ - (i_{X/M})_* \sum_k (-1)^k C_T(E_k, N_{X/M})\end{aligned}$$

We can simplify the formula of proposition 8.21 if we assume that our theory of singular Bott-Chern classes is compatible with the projection formula.

Corollary 8.22. *With the hypothesis of proposition 8.21, assume furthermore that T is compatible with the projection formula. Then*

$$\begin{aligned}T(\overline{\xi}_{Y\hookrightarrow M}) = \sum_k (-1)^k T(\overline{\xi}_{X\hookrightarrow M,k}) + (i_{X/M})_*(T(\overline{\xi}_{Y\hookrightarrow X}) \bullet \operatorname{Td}^{-1}(\overline{N}_{X/M}))\\ + (i_{Y/M})_* \operatorname{ch}(\overline{F}) \bullet \widetilde{\operatorname{Td}^{-1}}(\overline{\varepsilon}_N)\\ + (i_{Y/M})_* \Big[C_T^{\mathrm{ad}}(F, N_{Y/X}, i_{Y/X}^* N_{X/M}) - C_T(F, N_{Y/X}) \bullet \operatorname{Td}^{-1}(i_{Y/X}^* N_{X/M}))\\ - C_T(F, i_{Y/X}^* N_{X/M}) \bullet \operatorname{Td}^{-1}(N_{Y/X})\Big]\end{aligned}$$

Proof. Since T is compatible with the projection formula, then C_T is also. Therefore, using the Grothendieck-Riemann-Roch theorem for closed immersions at the level of analytic Deligne cohomology classes, we have

$$\begin{aligned}\sum_k (-1)^k C_T(E_k, N_{X/M}) &= C_T(\mathcal{O}_X, N_{X/M}) \bullet \sum_k (-1)^k \operatorname{ch}(E_k)\\ &= C_T(\mathcal{O}_X, N_{X/M}) \bullet (i_{Y/X})_*(\operatorname{ch}(F) \bullet \operatorname{Td}^{-1}(N_{Y/X}))\\ &= (i_{Y/X})_*(i_{Y/X}^* C_T(\mathcal{O}_X, N_{X/M}) \bullet \operatorname{ch}(F) \bullet \operatorname{Td}^{-1}(N_{Y/X}))\\ &= (i_{Y/X})_*(C_T(F, i_{Y/X}^* N_{X/M}) \bullet \operatorname{Td}^{-1}(N_{Y/X})),\end{aligned}$$

which implies the result. □

Definition 8.23. Let T be a theory of singular Bott-Chern classes. We will say that T is *transitive* if the equation

$$T(\overline{\xi}_{Y\hookrightarrow M}) = \sum_k (-1)^k T(\overline{\xi}_{X\hookrightarrow M,k}) + (i_{X/M})_*(T(\overline{\xi}_{Y\hookrightarrow X}) \bullet \operatorname{Td}^{-1}(\overline{N}_{X/M})) \\ + (i_{Y/M})_* \operatorname{ch}(\overline{F}) \bullet \widetilde{\operatorname{Td}^{-1}}(\overline{\varepsilon}_N) \quad (8.24)$$

holds. When equation (8.24) is satisfied for a particular choice of complex immersions and resolutions, we say that the theory T is *transitive with respect to this particular choice.*

We now introduce an abstract version of definition 8.17.

Definition 8.25. Given any characteristic class C of pairs of vector bundles, we will denote

$$C^{\rho}(F, N_1, N_2) := C(F, N_1 \oplus N_2) - \rho(F, N_1, N_2),$$

where ρ is the characteristic class of definition 8.17.

Note that, when T is a theory of singular Bott-Chern classes we have

$$C^{\rho}_T(F, N_1, N_2) = C^{\mathrm{ad}}_T(F, N_1, N_2).$$

Definition 8.26. We will say that a characteristic class C (of pairs of vector bundles) is *ρ-Todd additive* (in the second variable) if it satisfies

$$C(F, N_1 \oplus N_2) = C(F, N_1) \bullet \operatorname{Td}^{-1}(N_2) + C(F, N_2) \bullet \operatorname{Td}^{-1}(N_1) + \rho(F, N_1, N_2)$$

or, equivalently,

$$C^{\rho}(F, N_1, N_2) = C(F, N_1) \bullet \operatorname{Td}^{-1}(N_2) + C(F, N_2) \bullet \operatorname{Td}^{-1}(N_1).$$

A direct consequence of corollary 8.22 is

Corollary 8.27. *Let T be a theory of singular Bott-Chern classes that is compatible with the projection formula. Then it is transitive if and only if the associated characteristic class C_T is ρ-Todd additive.*

Since we are mainly interested in singular Bott-Chern classes that are transitive and compatible with the projection formula, we will study characteristic classes that are compatible with the projection formula and ρ-Todd-additive in the second variable. Since we want to express any characteristic class in terms of a power series we will restrict ourselves to the algebraic category.

Proposition 8.28. *Let C be a class that is compatible with the projection formula and ρ-Todd additive in the second variable. Then C determines a power series $\phi_C(x)$ given by*

$$C(\mathcal{O}_Y, L) = \phi_C(c_1(L)), \quad (8.29)$$

for every complex algebraic manifold Y and algebraic line bundle Y. Conversely, given any power series in one variable $\phi(x)$, there exists a unique characteristic class for algebraic vector bundles that is compatible with the projection formula and ρ-Todd additive in the second variable such that equation (8.29) *holds.*

Proof. This result follows directly from the splitting principle and theorem 1.8. □

Remark 8.30. The utility of corollary 8.27 and proposition 8.28 is limited by the fact that we do not know an explicit formula for the class $\rho(\mathcal{O}_Y, N_1, N_2)$. This class is related with the arithmetic difference between $\mathbb{P}_Y(N_1 \oplus N_2 \oplus \mathbb{C})$ and $\mathbb{P}_Y(N_1 \oplus \mathbb{C}) \underset{Y}{\times} \mathbb{P}_Y(N_2 \oplus \mathbb{C})$, the second space being simpler than the first. The main ingredients needed to compute this class are the Bott-Chern classes of the tautological exact sequence. Therefore the work of Mourougane [29] might be useful for computing this class.

Recall that an additive genus is a characteristic class for algebraic vector bundles S such that

$$S(N_1 \oplus N_2) = S(N_1) + S(N_2).$$

Let $\phi(x) = \sum_{i=0}^{\infty} a_i x^i$ be a power series in one variable. There is a one to one correspondence between additive genus and power series characterized by the condition that $S(L) = \phi(c_1(L))$, for each line bundle L.
Since the class ρ does not depend on the theory T it cancels out when considering the difference between two different theories of singular Bott-Chern classes.

Proposition 8.31. *Let C_1 and C_2 be two characteristic classes for pairs of algebraic vector bundles that are compatible with the projection formula and ρ-Todd-additive in the second variable. Then there is a unique additive genus S_{12} such that*

$$C_1(F, N) - C_2(F, N) = \mathrm{ch}(F) \bullet \mathrm{Td}(N)^{-1} \bullet S_{12}(N). \tag{8.32}$$

We can summarize the results of this section in the following theorem.

Theorem 8.33. *There is a one to one correspondence between theories of singular Bott-Chern classes for complex algebraic manifolds that are transitive and compatible with the projection formula, and formal power series $\phi(x) \in \mathbb{R}[[x]]$. To each theory of singular Bott-Chern classes corresponds the power series ϕ such that*

$$C_T(\mathcal{O}_Y, L) = \mathbf{1}_1 \bullet \phi(c_1(L)), \tag{8.34}$$

for every complex algebraic manifold Y and every algebraic line bundle L. To each power series ϕ it corresponds a unique class C, compatible with the projection formula and ρ-Todd-additive in the second variable, characterized by equation (8.34) *and a theory of singular Bott-Chern given by definition 7.4.*

Even if we do not know the exact value of the class ρ another consequence of corollary 8.27 is that, in order to prove the transitivity of a theory of singular Bott-Chern classes it is enough to check it for a particular class of compositions.

Corollary 8.35. *Let T be a theory of singular Bott-Chern classes compatible with the projection formula. Then T is transitive if and only if for any compact complex manifold Y and vector bundles N_1, N_2, the theory T is transitive with respect to the composition of inclusions*

$$Y \hookrightarrow \mathbb{P}_Y(N_1 \oplus \mathbb{C}) \hookrightarrow \mathbb{P}_Y(N_1 \oplus \mathbb{C}) \times_Y \mathbb{P}_Y(N_2 \oplus \mathbb{C})$$

and the Koszul resolutions. □

We can make the previous corollary a little more explicit. Let π_1 and π_2 be the projections from $P := \mathbb{P}_Y(N_1 \oplus \mathbb{C}) \times_Y \mathbb{P}_Y(N_2 \oplus \mathbb{C})$ to $P_1 := \mathbb{P}_Y(N_1 \oplus \mathbb{C})$ and $P_2 := \mathbb{P}_Y(N_2 \oplus \mathbb{C})$ respectively. Let $\overline{K}_1 = K(\overline{\mathcal{O}}_Y, \overline{N}_1)$ and $\overline{K}_2 = K(\overline{\mathcal{O}}_Y, \overline{N}_2)$ be the Koszul resolutions in P_1 and P_2 respectively. Then,

$$\overline{K} = \pi_1^* K_1 \otimes \pi_2^* K_2$$

is a resolution of $\mathcal{O}_Y$ in P. Then the theory T is transitive in this case if

$$T(\overline{K}) = \pi_2^* T(\overline{K}_2) \bullet \pi_1^*(c_{r_1}(\overline{Q}_1) \bullet \operatorname{Td}^{-1}(\overline{Q}_1)) + (i_1)_*(T(\overline{K}_1) \bullet p_1^* \operatorname{Td}^{-1}(\overline{N}_2)),$$

where r_1 is the rank of N_1, $\overline{Q}_1$ is the tautological quotient bundle in P_1 with the induced metric, $i_1 \colon P_1 \longrightarrow P$ is the inclusion and $p_1 \colon P_1 \longrightarrow Y$ is the projection.

The singular Bott-Chern classes that we have defined depend on the choice of a hermitian metric on the normal bundle and behave well with respect inverse images. Nevertheless, when one is interested in covariant functorial properties and, in particular, in a composition of closed immersions, it might be interesting to consider a variant of singular Bott-Chern classes that depend on the choice of metrics on the tangent bundles to Y and X.

Notation 8.36. Let $\overline{\xi} = (i \colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_* \to i_*F)$ be a hermitian embedded vector bundle. Let $\overline{T}_X$ and $\overline{T}_Y$ be the tangent bundles to X and Y provided with hermitian metrics. As usual we write $\operatorname{Td}(Y) = \operatorname{Td}(\overline{T}_Y)$ and $\operatorname{Td}(X) = \operatorname{Td}(\overline{T}_X)$. We put

$$\overline{\xi}_c = (i \colon Y \longrightarrow X, \overline{T}_X, \overline{T}_Y, \overline{F}, \overline{E}_* \to i_*F).$$

By abuse of notation we will also say that $\overline{\xi}_c$ is a hermitian embedded vector bundle. In this situation we denote by $\overline{\xi}_{N_{Y/X}}$ the exact sequence of hermitian vector bundles

$$\overline{\xi}_{N_{Y/X}} \colon 0 \longrightarrow \overline{T}_Y \longrightarrow i^*\overline{T}_X \longrightarrow \overline{N}_{Y/X} \longrightarrow 0.$$

If there is no danger of confusion we will denote $\overline{N} = \overline{N}_{Y/X}$ and therefore $\overline{\xi}_N = \overline{\xi}_{N_{Y/X}}$.

Definition 8.37. Let T be a theory of singular Bott-Chern classes. Then the *covariant singular Bott-Chern class* associated to T is given by

$$T_c(\overline{\xi}_c) = T(\overline{\xi}) + i_*(\operatorname{ch}(\overline{F}) \bullet \widetilde{\operatorname{Td}^{-1}}(\overline{\xi}_{N_{Y/X}}) \operatorname{Td}(Y)) \tag{8.38}$$

Proposition 8.39. *The covariant singular Bott-Chern classes satisfy the following properties*

(i) The class $T_c(\overline{\xi}_c)$ does not depend on the choice of the metric on $N_{Y/X}$.

(ii) The differential equation

$$\mathrm{d}_{\mathcal{D}} T_c(\overline{\xi}_c) = \sum_k (-1)^k \operatorname{ch}(\overline{E}_k) - i_*(\operatorname{ch}(\overline{F}) \bullet \operatorname{Td}(Y)) \bullet \operatorname{Td}^{-1}(X) \tag{8.40}$$

holds.

(iii) If the theory T is compatible with the projection formula, then

$$T_c(\overline{\xi}_c \otimes \overline{G}) = T_c(\overline{\xi}_c) \bullet \operatorname{ch}(\overline{G}).$$

(iv) If, moreover, the theory T is transitive, then, using notation 8.8 adapted to the current setting, we have

$$\begin{aligned} T_c(\overline{\xi}_{Y \hookrightarrow M,c}) = &\sum_k (-1)^k T_c(\overline{\xi}_{X \hookrightarrow M,k,c}) \\ &+ (i_{X/M})_*(T_c(\overline{\xi}_{Y \hookrightarrow X,c}) \bullet \operatorname{Td}(X)) \bullet \operatorname{Td}^{-1}(M). \end{aligned} \tag{8.41}$$

(v) With the hypothesis of corollary 6.14, we have

$$T_c(\bigoplus_{j \text{ even}} \overline{\xi}_{j,c}) - T_c(\bigoplus_{j \text{ odd}} \overline{\xi}_{j,c}) = [\widetilde{\operatorname{ch}}(\overline{\varepsilon})] - i_*([\widetilde{\operatorname{ch}}(\overline{\chi}) \bullet \operatorname{Td}(Y)]) \bullet \operatorname{Td}^{-1}(X). \tag{8.42}$$

Proof. All the statements follow from straightforward computations. □

9 Homogeneous singular Bott-Chern classes

In this section we will show that, by adding a natural fourth axiom to definition 6.9, we obtain a unique theory of singular Bott-Chern classes that we call homogeneous singular Bott-Chern classes, and we will compare it with the classes previously defined by Bismut, Gillet and Soulé and by Zha.
In the paper [6], Bismut, Gillet and Soulé introduced a theory of singular Bott-Chern classes that is the main ingredient in their construction of direct images for closed immersions.
Strictly speaking, the construction of [6] only produces a theory of singular Bott-Chern classes in the sense of this paper when the metrics involved satisfy

a technical condition, called Condition (A) of Bismut. Nevertheless, there is a unique way to extend the definition of [6] from metrics satisfying Bismut's condition (A) to general metrics in such a way that one obtains a theory of singular Bott-Chern classes in the sense of this paper.
In his thesis [32], Zha gave another definition of singular Bott-Chern classes, and he also used them to define direct images for closed immersions in Arakelov theory.
We will recall the construction of both theories of singular Bott-Chern classes and we will show that they agree with the theory of homogeneous singular Bott-Chern classes.
We warn the reader that the normalizations we use differ from the normalizations in [6] and [32]. The main difference is that we insist on using the algebro-geometric twist in cohomology, whereas in the other two papers the authors use cohomology with real coefficients.
Let r_F and r_N be two positive integers. Let Y be a complex manifold and let $\overline{F}$ and $\overline{N}$ be two hermitian vector bundles of rank r_F and r_N respectively. Let $P = \mathbb{P}(N \oplus \mathbb{C})$ and let s be the zero section. We will follow the notations of definition 5.3. Then $T(K(\overline{F}, \overline{N}))$ satisfies the differential equation

$$\mathrm{d}_{\mathcal{D}}\, T(K(\overline{F}, \overline{N})) = c_{r_N}(\overline{Q})\, \mathrm{Td}^{-1}(\overline{Q})\, \mathrm{ch}(\pi_P^* \overline{F}) - s_*(\mathrm{ch}(\overline{F})\, \mathrm{Td}^{-1}(\overline{N})).$$

Therefore, the class

$$\widetilde{e}_T(\overline{F}, \overline{N}) := T(K(\overline{F}, \overline{N})) \bullet \mathrm{Td}(\overline{Q}) \bullet \mathrm{ch}^{-1}(\pi_P^* \overline{F})$$

satisfies the simpler equation

$$\mathrm{d}_{\mathcal{D}}\, \widetilde{e}_T(\overline{F}, \overline{N}) = [c_{r_N}(\overline{Q})] - \delta_Y. \tag{9.1}$$

Observe that the right hand side of this equation belongs to $\mathcal{D}_D^{2r_N}(P, r_N)$. Thus it seems natural to introduce the following definition.

Definition 9.2. Let T be a theory of singular Bott-Chern classes of rank $r_F > 0$ and codimension r_N. Then the class

$$\widetilde{e}_T(\overline{F}, \overline{N}) = T(K(\overline{F}, \overline{N})) \bullet \mathrm{Td}(\overline{Q}) \bullet \mathrm{ch}^{-1}(\pi_P^* \overline{F})$$

is called the *Euler-Green class associated to T*. The class $T(K(\overline{F}, \overline{N}))$ is said to be *homogeneous* if

$$\widetilde{e}_T(\overline{F}, \overline{N}) \in \widetilde{\mathcal{D}}_D^{2r_N - 1}(P, r_N).$$

A theory of singular Bott-Chern classes of rank 0 is said to be *homogeneous* if it agrees with the theory of Bott-Chern classes associated to the Chern character. Finally, a theory of singular Bott-Chern classes is said to be *homogeneous* if its restrictions to all ranks and codimensions are homogeneous.

The main interest of the above definition is the following result.

Theorem 9.3. *Given two positive integers r_F and r_N there exists a unique theory of homogeneous singular Bott-Chern classes of rank r_F and codimension r_N.*

Proof. The proof of this result is based on the theory of Euler-Green classes. Let $P = \mathbb{P}(N \oplus \mathbb{C})$ be as before, and let s denote the zero section of P. Let D_∞ be the subvariety of P that parametrizes the lines contained in N. Then $D_\infty = \mathbb{P}(N)$.

Lemma 9.4. *There exists a unique class $\widetilde{e}(P, \overline{Q}, s) \in \mathcal{D}^{2r_N-1}_D(P, r_N)$ such that*

(i) It satisfies

$$\mathrm{d}_{\mathcal{D}}\, \widetilde{e}(P, \overline{Q}, s) = [c_{r_N}(\overline{Q})] - \delta_Y. \tag{9.5}$$

(ii) The restriction $\widetilde{e}(P, \overline{Q}, s)|_{D_\infty} = 0$.

Proof. We first show the uniqueness. Assume that $\widetilde{e}$ and $\widetilde{e}'$ are two classes that satisfy the hypothesis of the theorem. Then $\widetilde{e}' - \widetilde{e}$ is closed. Hence it determines a cohomology class in $H^{2r_N-1}_{\mathcal{D}^{\mathrm{an}}}(P, r_N)$. Since, by theorem 1.2, the restriction

$$H^{2r_N-1}_{\mathcal{D}^{\mathrm{an}}}(P, r_N) \longrightarrow H^{2r_N-1}_{\mathcal{D}^{\mathrm{an}}}(D_\infty, r_N) \tag{9.6}$$

is an isomorphism, condition (ii) implies that $\widetilde{e}' = \widetilde{e}$. Now we prove the existence. Since Y is the zero locus of the section s, that is transversal to the zero section of Q, we know that the currents $[c_{r_N}]$ and δ_Y are cohomologous. Therefore there exists an element $\widetilde{a} \in \widetilde{\mathcal{D}}^{2r_N-1}_D(P, r_N)$ such that $\mathrm{d}_{\mathcal{D}}\, \widetilde{a} = [c_{r_N}(\overline{Q})] - \delta_Y$. Since $\overline{Q}$ restricted to D_∞ splits as an orthogonal direct sum

$$\overline{Q}|_{D_\infty} = \overline{S} \oplus \overline{\mathbb{C}} \tag{9.7}$$

where the metric on the factor $\mathbb{C}$ is trivial, and the section s restricts to the constant section 1, we obtain that $([c_{r_N}(\overline{Q})] - \delta_Y)|_{D_\infty} = 0$. Therefore $\widetilde{a}$ determines a class in $H^{2r_N-1}_{\mathcal{D}^{\mathrm{an}}}(P, r_N)$. Using again that (9.6) is an isomorphism, we find an element $\widetilde{b} \in H^{2r_N-1}_{\mathcal{D}^{\mathrm{an}}}(P, r_N)$, such that $\widetilde{e} = \widetilde{a} - \widetilde{b}$ satisfies the conditions of the lemma. □

We continue with the proof of theorem 9.3. We first prove the uniqueness. Let T be a theory of homogeneous singular Bott-Chern classes. The splitting (9.7) implies easily that the restriction of the Koszul resolution $K(\overline{F}, \overline{N})$ to D_∞ is orthogonally split. By the functoriality of singular Bott-Chern classes, $T(K(\overline{F}, \overline{N}))|_{D_\infty} = 0$. Thus the class

$$\widetilde{e}_T(\overline{F}, \overline{N}) := T(K(\overline{F}, \overline{N})) \bullet \mathrm{Td}(\overline{Q}) \bullet \mathrm{ch}^{-1}(\pi_P^* \overline{F}) \in \widetilde{\mathcal{D}}^{2r_N-1}_D(P, r_N)$$

satisfies the two conditions of lemma 9.4. Therefore $\widetilde{e}_T(\overline{F}, \overline{N}) = \widetilde{e}(P, \overline{Q}, s)$ and

$$T(K(\overline{F}, \overline{N})) = \widetilde{e}(P, \overline{Q}, s) \bullet \mathrm{Td}^{-1}(\overline{Q}) \bullet \mathrm{ch}(\pi_P^* \overline{F}), \tag{9.8}$$

where the right hand side does not depend on the theory T. In consequence we have that

$$C_T(F,N) = (\pi_P)_* T(K(\overline{F},\overline{N})) \tag{9.9}$$

does not depend on the theory T. Thus by the uniqueness in theorem 7.1 we obtain the uniqueness here.
For the existence we observe

Lemma 9.10. *The current*

$$C(F,N) = (\pi_P)_*(\widetilde{e}(P,\overline{Q},s) \bullet \mathrm{Td}^{-1}(\overline{Q})) \bullet \mathrm{ch}(\overline{F})$$

is a characteristic class for pairs of vector bundles of rank r_F and r_N.

Proof. We first compute, using equation (9.5) and corollary 3.8,

$$\begin{aligned} \mathrm{d}_{\mathcal{D}} C(F,N) &= (\pi_P)_* \left(\mathrm{d}_{\mathcal{D}} \widetilde{e}(P,\overline{Q},s) \bullet \mathrm{Td}^{-1}(\overline{Q})\right) \bullet \mathrm{ch}(\overline{F}) \\ &= (\pi_P)_* \left(([c_{r_N}(\overline{Q})] - \delta_Y) \bullet \mathrm{Td}^{-1}(\overline{Q})\right) \bullet \mathrm{ch}(\overline{F}) \\ &= (\pi_P)_* \left(c_{r_N}(\overline{Q}) \bullet \mathrm{Td}^{-1}(\overline{Q})\right) \bullet \mathrm{ch}(\overline{F}) - \mathrm{Td}^{-1}(\overline{N}) \bullet \mathrm{ch}(\overline{F}) \\ &= 0. \end{aligned}$$

Thus $C(F,N)$ determines a cohomology class. This class is functorial by construction. By proposition 1.7 this class does not depend on the metric and defines a characteristic class. □

By the existence in theorem 7.1 we obtain a theory of singular Bott-Chern classes T_C that is easily seen to be homogeneous. □

A reformulation of theorem 9.3 is

Theorem 9.11. *There exists a unique way to associate to each hermitian embedded vector bundle $\overline{\xi} = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_*)$ a class of currents*

$$T^h(\overline{\xi}) \in \bigoplus_p \widetilde{\mathcal{D}}_D^{2p-1}(X, N^*_{Y,0}, p)$$

that we call homogeneous singular Bott-Chern class, satisfying the following properties

(i) *(Differential equation) The equality*

$$\mathrm{d}_{\mathcal{D}} T^h(\overline{\xi}) = \sum_i (-1)^i [\mathrm{ch}(\overline{E}_i)] - i_*([\mathrm{Td}^{-1}(\overline{N})\,\mathrm{ch}(\overline{F})]) \tag{9.12}$$

holds.

(ii) *(Functoriality) For every morphism $f\colon X' \longrightarrow X$ of complex manifolds that is transverse to Y,*

$$f^* T^h(\overline{\xi}) = T^h(f^*\overline{\xi}).$$

(iii) *(Normalization) Let $\overline{A}=(A_*,g_*)$ be a non-negatively graded orthogonally split complex of vector bundles. Write $\overline{\xi}\oplus\overline{A}=(i\colon Y\longrightarrow X,\overline{N},\overline{F},\overline{E}_*\oplus\overline{A}_*)$. Then $T^h(\overline{\xi})=T^h(\overline{\xi}\oplus\overline{A})$. Moreover, if $X=\operatorname{Spec}\mathbb{C}$ is one point, $Y=\emptyset$ and $\overline{E}_*=0$, then $T^h(\overline{\xi})=0$.*

(iv) *(Homogeneity) If $r_F=\operatorname{rk}(F)>0$ and $r_N=\operatorname{rk}(N)>0$, then, with the notations of definition 9.2,*

$$T^h(K(\overline{F},\overline{N}))\bullet\operatorname{Td}(\overline{Q})\bullet\operatorname{ch}^{-1}(\pi_P^*\overline{F})\in\widetilde{\mathcal{D}}_D^{2r_N-1}(P,r_N).$$

□

The class $\widetilde{e}(P,\overline{Q},s)$ of lemma 9.4 is a particular case of the Euler-Green classes introduced by Bismut, Gillet and Soulé in [6]. The basic properties of the Euler-Green classes are summarized in the following results.

Proposition 9.13. *Let X be a complex manifold, let $\overline{E}$ be a hermitian holomorphic vector bundle of rank r and let s be a holomorphic section of E that is transverse to the zero section. Denote by Y the zero locus of s. There is a unique way to assign to each $(X,\overline{E},s)$ as before a class of currents*

$$\widetilde{e}(X,\overline{E},s)\in\widetilde{\mathcal{D}}_D^{2r-1}(X,N^*_{Y,0},r)$$

satisfying the following properties

(i) *(Differential equation)*

$$\mathrm{d}_{\mathcal{D}}\,\widetilde{e}(X,\overline{E},s)=c_r(\overline{E})-\delta_Y. \tag{9.14}$$

(ii) *(Functoriality) If $f\colon X'\longrightarrow X$ is a morphism transverse to Y then*

$$\widetilde{e}(X',f^*\overline{E},f^*s)=f^*\widetilde{e}(X,\overline{E},s). \tag{9.15}$$

(iii) *(Multiplicativity) Let $\overline{E}_1$ and $\overline{E}_2$ be hermitian holomorphic vector bundles, and let s_1 and s_2 be holomorphic sections of $\overline{E}_1$ and $\overline{E}_2$ respectively that are transverse to the zero section and with zero locus Y_1 and Y_2. We write $\overline{E}=\overline{E}_1\oplus\overline{E}_2$ and $s=s_1\oplus s_2$. Assume that s is transverse to the zero section; hence Y_1 and Y_2 meet transversely. With this hypothesis we have*

$$\begin{aligned}\widetilde{e}(X,\overline{E},s)&=\widetilde{e}(X,\overline{E}_1,s_1)\wedge c_{r_2}(\overline{E}_2)+\delta_{Y_1}\wedge\widetilde{e}(X,\overline{E}_2,s_2)\\&=\widetilde{e}(X,\overline{E}_1,s_1)\wedge\delta_{Y_2}+c_{r_1}(\overline{E}_1)\wedge\widetilde{e}(X,\overline{E}_2,s_2).\end{aligned}$$

(iv) *(Line bundles) If $\overline{L}$ is a hermitian line bundle and s is a section of L, then*

$$\widetilde{e}(X,\overline{L},s)=-\log\|s\|. \tag{9.16}$$

Proof. Bismut, Gillet and Soulé prove the existence by constructing explicitly an Euler-Green current in the total space of E and pulling it back to X by the section s. For the uniqueness, first we see that properties (i) and (ii) imply that, if h_0 and h_1 are two hermitian metrics in E, then

$$\widetilde{e}(X,(E,h_0),s)-\widetilde{e}(X,(E,h_1),s)=\widetilde{c}_r(E,h_0,h_1). \tag{9.17}$$

We now consider $\pi\colon P=\mathbb{P}(E\oplus\mathbb{C})\longrightarrow X$, with the tautological exact sequence

$$0\longrightarrow\mathcal{O}(-1)\longrightarrow\pi^*E\oplus\mathbb{C}\longrightarrow Q\longrightarrow 0$$

On Q we consider the metric induced by the metric of $\overline{E}$ and the trivial metric on the factor $\mathbb{C}$, and let s_Q the section of Q induced by the section 1 of $\mathbb{C}$. Let D_∞ be as in lemma 9.4. Then properties (ii) to (iv) imply that $\widetilde{e}(P,\overline{Q},s_Q)|_{D_\infty}=0$. Hence by lemma 9.4 $\widetilde{e}$ is uniquely determined. Finally, let $f\colon X\longrightarrow P$ be the map given by $x\longmapsto(s(x):-1)$. Then $f^*Q\cong E$, although they are not necessarily isometric, and $f^*s_Q=s$. Therefore, the functoriality and equation (9.17) determine $\widetilde{e}(X,\overline{E},s)$.

To prove the existence, we use lemma 9.4, functoriality and equation (9.17) to define the Euler-Green classes. It is easy to show that they are well defined and satisfy properties (i) to (iv). □

Equation (9.8) relating homogeneous singular Bott-Chern classes and Euler-Green classes in a particular case can be generalized to arbitrary vector bundles.

Proposition 9.18. *Let X be a complex manifold, $\overline{E}$ a hermitian vector bundle over X, s a section of E transversal to the zero section and $i\colon Y\longrightarrow X$ the zero locus of s. Let $K(\overline{E})$ be the Koszul resolution of $i_*\mathcal{O}_Y$ determined by $\overline{E}$ and s. We can identify $N_{Y/X}$ with i^*E. We denote by $\overline{N}_{Y/X}$ the vector bundle with the metric induced by the above identification. Then*

$$T^h(i,\overline{\mathcal{O}}_Y,\overline{N}_{Y/X},K(\overline{E}))=\widetilde{e}(X,\overline{E},s)\bullet\operatorname{Td}^{-1}(\overline{E}).$$

Proof. Let $P=\mathbb{P}(E\oplus\mathbb{C})$. We follow the notation of proposition 9.13. We denote by h_0 the original metric of $\overline{E}$ and by h_1 the metric induced by the isomorphism $E\cong f^*Q$. Observe that h_0 and h_1 agree when restricted to Y, because the preimage of $\overline{Q}$ by the zero section agrees with $\overline{E}$. Hence there is an isometry $\overline{N}_{Y/X}\cong i^*f^*\overline{Q}$. We denote $T^h(K(\overline{E}))=T^h(i,\overline{\mathcal{O}}_Y,\overline{N}_{Y/X},K(\overline{E}))$.

Then we have

$$\begin{aligned}
T^h(K(\overline{E})) &= f^*T^h(K(\overline{\mathcal{O}_X},\overline{E})) + \sum_i (-1)^i \widetilde{\mathrm{ch}}(\bigwedge^i E^\vee, h_0, h_1)\\
&= f^*(\widetilde{e}(P,\overline{Q},s_Q)\bullet \mathrm{Td}^{-1}(\overline{Q})) + \widetilde{c}_r(E,h_0,h_1)\bullet \mathrm{Td}^{-1}(E,h_1)\\
&\qquad + c_r(E,h_0)\bullet \widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)\\
&= \widetilde{e}(X,\overline{E},s)\bullet \mathrm{Td}^{-1}(E,h_1) - \widetilde{c}_r(E,h_0,h_1)\bullet \mathrm{Td}^{-1}(E,h_1)\\
&\qquad + \widetilde{c}_r(E,h_0,h_1)\bullet \mathrm{Td}^{-1}(E,h_1) + c_r(E,h_0)\bullet \widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)\\
&= \widetilde{e}(X,\overline{E},s)\bullet \mathrm{Td}^{-1}(E,h_0) - \widetilde{e}(X,\overline{E},s)\bullet \mathrm{d}_{\mathcal{D}}\widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)\\
&\qquad + c_r(E,h_0)\bullet \widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)\\
&= \widetilde{e}(X,\overline{E},s)\bullet \mathrm{Td}^{-1}(E,h_0) - \mathrm{d}_{\mathcal{D}}\widetilde{e}(X,\overline{E},s)\bullet \widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)\\
&\qquad + c_r(E,h_0)\bullet \widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)\\
&= \widetilde{e}(X,\overline{E},s)\bullet \mathrm{Td}^{-1}(E,h_0) + i_*\widetilde{\mathrm{Td}^{-1}}(E,h_0,h_1)|_Y\\
&= \widetilde{e}(X,\overline{E},s)\bullet \mathrm{Td}^{-1}(\overline{E}),
\end{aligned}$$

which concludes the proof. □

Theorem 9.19. *The theory of homogeneous singular Bott-Chern classes is compatible with the projection formula and transitive.*

Proof. We have

$$\begin{aligned}
C_{T^h}(F,N) &= (\pi_P)_*T^h(K(\overline{F},\overline{N}))\\
&= (\pi_P)_*(\widetilde{e}(P,\overline{Q},s)\bullet \mathrm{Td}^{-1}(\overline{Q})\bullet \mathrm{ch}(\pi_P^*\overline{F}))\\
&= (\pi_P)_*(\widetilde{e}(P,\overline{Q},s)\bullet \mathrm{Td}^{-1}(\overline{Q}))\bullet \mathrm{ch}(\overline{F})\\
&= C_{T^h}(\mathcal{O}_Y,N)\bullet \mathrm{ch}(F).
\end{aligned}$$

Thus C_{T^h} is compatible with the projection formula.
We now prove the transitivity. Let Y, N_1 and N_2 be as in corollary 8.35. We follow the notation after this corollary. Then applying proposition 9.18 we obtain

$$T^h(\overline{K}) = \widetilde{e}(P,\pi_1^*\overline{Q}_1\oplus\pi_2^*\overline{Q}_2, s_1+s_2)\bullet \mathrm{Td}^{-1}(\pi_1^*\overline{Q}_1\oplus\pi_2^*\overline{Q}_2), \tag{9.20}$$

where s_i denote the tautological section of $\overline{Q}_i$ or its preimage by π_i.
Then, by proposition 9.13 (iii), taking into account that $Y_1 = P_2$,

$$\begin{aligned}
T^h(\overline{K}) = \pi_1^*(c_{r_1}(\overline{Q}_1)\,\mathrm{Td}^{-1}(\overline{Q}_1))\bullet \pi_2^*(\widetilde{e}(P_2,\overline{Q}_2,s_2)\,\mathrm{Td}^{-1}(\overline{Q}_2))\\
+ (i_1)_*(\widetilde{e}(P_1,\overline{Q}_1,s_1)\,\mathrm{Td}^{-1}(\overline{Q}_1)\bullet p_1^*\,\mathrm{Td}^{-1}(\overline{N}_2)).
\end{aligned} \tag{9.21}$$

Applying again proposition 9.18 we obtain

$$T^h(\overline{K}) = \pi_1^*(c_{r_1}(\overline{Q}_1)\operatorname{Td}^{-1}(\overline{Q}_1)) \bullet \pi_2^*(T^h(\overline{K}_2)) + (i_1)_*(T^h(\overline{K}_1) \bullet p_1^* \operatorname{Td}^{-1}(\overline{N}_2)). \tag{9.22}$$

Thus, by corollary 8.35 the theory of homogeneous singular Bott-Chern classes is transitive. □

We next recall the construction of singular Bott-Chern classes of Bismut, Gillet and Soulé. Let $i\colon Y \longrightarrow X$ be a closed immersion of complex manifolds and let $\overline{\xi} = (i, \overline{N}, \overline{F}, \overline{E}_*)$ be a hermitian embedded vector bundle. We consider the associated complex of sheaves

$$0 \to E_n \xrightarrow{v} \dots \xrightarrow{v} E_0 \to 0,$$

where we denote by v the differential of this complex.
This complex is exact for all $x \in X \setminus Y$. The cohomology sheaves of this complex are holomorphic vector bundles on Y which we denote by

$$H_n = \mathcal{H}_n(E_*|_Y), \quad H = \bigoplus_n H_n.$$

For each $x \in Y$ and $U \in T_xX$ we denote by $\partial_U v(x)$ the derivative of the map v calculated in any holomorphic trivialization of E near x. Then $\partial_U v(x)$ acts on H_x. Moreover, this action only depends on the class y of U in N_x. We denote it by $\partial_y v(x)$. Moreover $(\partial_y v(x))^2 = 0$; therefore the pull-back of H to the total space of N together with $\partial_y v$ is a complex that we denote by $(H, \partial_y v)$.
On the total space of N, the interior multiplication by $y \in N$ turns $\bigwedge N^\vee$ into a Koszul complex. By abuse of notation we denote also by ι_y the operator $\iota_y \otimes 1$ acting on $\bigwedge N^\vee \otimes F$. There is a canonical isomorphism between the complexes $(H, \partial_y v)$ and $(\bigwedge N^\vee \otimes F, \iota_y)$. An explicit description of this isomorphism can be found in [3] §1.
Let v^* be the adjoint of the operator v with respect to the metrics of $\overline{E}_*$. Then we have an identification of vector bundles over Y

$$H_k = \{f \in E_k \mid vf = v^* f = 0\}.$$

This identification induces a hermitian metric on H_k, and hence on H. Note that the metrics on N and F also induce a hermitian metric on $\bigwedge N^\vee \otimes F$.

Definition 9.23. We say that $\overline{\xi} = (i, \overline{N}, \overline{F}, \overline{E}_*)$ satisfies Bismut assumption (A) if the canonical isomorphism between $(H, \partial_y v)$ and $(\bigwedge N^\vee \otimes F, \iota_y)$ is an isometry.

Proposition 9.24. *Let $\overline{\xi} = (i, \overline{N}, \overline{F}, \overline{E}_*)$ be as before, with $\overline{N} = (N, h_N)$ and $\overline{F} = (F, h_F)$. Then there exist metrics h'_{E_k} over E_k such that the hermitian embedded vector bundle $\overline{\xi}' = (i, \overline{N}, \overline{F}, (E_*, h'_{E_*}))$ satisfies Bismut assumption (A).*

Proof. This is [3] proposition 1.6. □

Let ∇^E be the canonical hermitian holomorphic connection on E and let $V = v + v^*$. Then

$$A_u = \nabla^E + \sqrt{u} V$$

is a superconnection on E.
Let ∇^H be the canonical hermitian connection on H. Then

$$B = \nabla^H + \partial_y v + (\partial_y v)^*$$

is a superconnection on H.
Let N_H be the number operator on the complex (E, v), that is, N_H acts on E_k by multiplication by k, and let Tr_s denote the supertrace. Recall that here we are using the symbol [ ] to denote the current associated to a locally integrable differential form and the symbol δ_Y to denote the current integration along a subvariety, both with the normalizations of notation 1.3.
For $0 < Re(s) \leq 1/2$ let $\zeta_E(s)$ be the current on X given by the formula

$$\zeta_E(s) = \frac{1}{\Gamma(s)} \int_0^\infty u^{s-1} \Big\{ \left[\mathrm{Tr}_s\left(N_H \exp(-A_u^2)\right)\right] \\ - i_* \left[\int_N \mathrm{Tr}_s\left(N_H \exp(-B^2)\right)\right] \Big\} \,\mathrm{d}\, u. \quad (9.25)$$

This current is well defined and extends to a current that depends holomorphically on s near 0.

Definition 9.26. Assume that $\overline{\xi} = (i, \overline{N}, \overline{F}, \overline{E}_*)$ satisfies Bismut assumption (A). Then we denote

$$T^{BGS}(\overline{\xi}) = -\frac{1}{2}\zeta_E'(0).$$

By abuse of notation we will denote also by $T^{BGS}(\overline{\xi})$ its class in $\widetilde{\bigoplus}_p \widetilde{\mathcal{D}}_D^{2p-1}(X, p)$.
Let now $\overline{\xi} = (i, \overline{N}, \overline{F}, (E_*, h_{E_*}))$ be general and let $\overline{\xi}' = (i, \overline{N}, \overline{F}, (E_*, h'_{E_*}))$ be any hermitian embedded vector bundle satisfying assumption (A) provided by proposition 9.24. Then we denote

$$T^{BGS}(\overline{\xi}) = T^{BGS}(\overline{\xi}') + \sum_i (-1)^i \widetilde{\mathrm{ch}}(E_i, h_{E_i}, h'_{E_i}),$$

where $\widetilde{\mathrm{ch}}(E_i, h_{E_i}, h'_{E_i})$ is as in definition 2.13.

Remark 9.27. This definition only agrees (up to a normalization factor) with the definition in [6] for hermitian embedded vector bundles that satisfy assumption (A).

Theorem 9.28. *The assignment that, to each hermitian embedded vector bundle $\overline{\xi}$, associates the current $T^{BGS}(\overline{\xi})$, is a theory of singular Bott-Chern classes that agrees with T^h.*

Proof. First we have to show that, when $\overline{\xi}$ does not satisfy assumption (A) then $T^{BGS}(\overline{\xi})$ is well defined. Assume that $\overline{\xi}'' = (i, \overline{N}, \overline{F}, (E_*, h'_{E_*}))$ is another choice of hermitian embedded vector bundle satisfying assumption (A). By lemma 2.17 we have that

$$\widetilde{\mathrm{ch}}(E_i, h_i, h'_i) + \widetilde{\mathrm{ch}}(E_i, h'_i, h''_i) + \widetilde{\mathrm{ch}}(E_i, h''_i, h_i) = 0.$$

By [6] theorem 2.5 we have that

$$T^{BGS}(\overline{\xi}') - T^{BGS}(\overline{\xi}'') = \sum_i (-1)^i \widetilde{\mathrm{ch}}(E_i, h'_{E_i}, h''_{E_i}).$$

Summing up we obtain that $T^{BGS}(\overline{\xi})$ is well defined.
If the hermitian embedded vector bundle $\overline{\xi}$ satisfies Bismut assumption (A) then, by [6] theorem 1.9, $T^{BGS}(\overline{\xi})$ satisfies equation (6.10). If $\overline{\xi}$ does not satisfy assumption (A) then, combining [6] theorem 1.9 and equation (2.4), we also obtain that $T^{BGS}(\overline{\xi})$ satisfies equation (6.10).
The functoriality property is [6] theorem 1.10.
In order to prove the normalization property, let $\overline{\xi} = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_*)$ be a hermitian embedded vector bundle that satisfies assumption (A) and let $\overline{A}$ be a non-negatively graded orthogonally split complex of vector bundles on X. Observe that $\overline{A}$ is also a (trivial) hermitian embedded vector bundle. Then $\overline{A}$ and $\overline{\xi} \oplus \overline{A}$ also satisfy assumption (A). By [6] theorem 2.9

$$T^{BGS}(\overline{\xi} \oplus \overline{A}) = T^{BGS}(\overline{\xi}) + T^{BGS}(\overline{A}).$$

But by [5] remark 2.3, $T^{BGS}(\overline{A})$ agrees with the Bott-Chern class associated to the Chern character and the exact complex $\overline{A}$. Since A is orthogonally split we have $T^{BGS}(\overline{A}) = 0$. Now the case when ξ does not satisfy assumption (A) follows from the definition.
By [6] theorem 3.17, with the hypothesis of proposition 9.18, we have that

$$\begin{aligned} T^{BGS}(i, \overline{\mathcal{O}}_Y, \overline{N}_{Y/X}, K(\overline{E})) &= \widetilde{e}(X, \overline{E}, s) \bullet \mathrm{Td}^{-1}(\overline{E}) \\ &= T^h(i, \overline{\mathcal{O}}_Y, \overline{N}_{Y/X}, K(\overline{E})). \end{aligned}$$

From this it follows that $C_{T^{BGS}} = C_{T^h}$ and by theorem 7.1, $T^{BGS} = T^h$. □

We now recall Zha's construction. Note that, in order to obtain a theory of singular Bott-Chern classes, we have changed the normalization convention from the one used by Zha. Note also that Zha does not define explicitly a singular Bott-Chern class, but such a definition is implicit in his definition of direct images for closed immersions. Let Y be a complex manifold and let $\overline{N} = (N, h)$ be a hermitian vector bundle. We denote $P = \mathbb{P}(N \oplus \mathbb{C})$. Let

$\pi\colon P \longrightarrow Y$ denote the projection and let $\iota\colon Y \longrightarrow P$ denote the inclusion as the zero section. On P we consider the tautological exact sequence

$$0 \longrightarrow \mathcal{O}(-1) \longrightarrow \pi^* N \oplus \mathcal{O}_P \longrightarrow Q \longrightarrow 0.$$

Let h_1 denote the hermitian metric on $Q^\vee$ induced by the metric of N and the trivial metric on $\mathcal{O}_P$ and let h_0 denote the semi-definite hermitian form on $Q^\vee$ induced by the map $Q^\vee \longrightarrow \mathcal{O}_P$ obtained from the above exact sequence and the trivial metric on $\mathcal{O}_P$. Let $h_t = (1-t^2)h_0 + t^2 h_1$. It is a hermitian metric on $Q^\vee$. We will denote $\overline{Q}_t^\vee = (Q^\vee, h_t)$. Let ∇_t be the associated hermitian holomorphic connection and let N_t denote the endomorphism defined by

$$\frac{\mathrm{d}}{\mathrm{d}\, t} \left\langle v, w \right\rangle_t = \left\langle N_t v, w \right\rangle .$$

For each $n \geq 1$, let Det denote the alternate n-linear form on the space of n by n matrices such that

$$\det(A) = \operatorname{Det}(A, \dots, A).$$

We denote $\det(B; A) = \operatorname{Det}(B, A, \dots, A)$.
Zha introduced the differential form

$$\widetilde{e}_Z(\overline{Q}^\vee) = \frac{-1}{2} \lim_{s \to 0} \int_s^1 \det(N_t, \nabla_t^2)\, \mathrm{d}\, t \tag{9.29}$$

which is a smooth form on $P \setminus \iota(Y)$, locally integrable on P. Hence it defines a current, also denoted by $\widetilde{e}_Z(\overline{Q}^\vee)$ on P. The important property of this current is that it satisfies

$$\mathrm{d}_{\mathcal{D}}\, \overline{e}_Z(Q^\vee) = c_n(\overline{Q}_1) - \delta_Y. \tag{9.30}$$

In [32], Zha denotes by $C(\overline{Q}^\vee)$ a form that differs from $\widetilde{e}_Z$ by the normalization factor and the sign. We denote it by $\widetilde{e}_Z$ because it agrees with the Euler-Green current introduced in [6].

Proposition 9.31. *The equality*

$$\widetilde{e}_Z(Q^\vee) = \widetilde{e}(P, \overline{Q}_1, s_Q)$$

holds.

Proof. With the notations of lemma 9.4, both classes satisfy equation (9.30) and their restriction to D_∞ is zero. By lemma 9.4 they agree. □

Definition 9.32. Let $\overline{\xi} = (i\colon Y \longrightarrow X, \overline{N}, \overline{F}, \overline{E}_*)$ be as in definition 6.9. Let $\overline{A}_*$, $\operatorname{tr}_1(\overline{E})_*$ and $\overline{\eta}_*$ be as in (7.2). Then we define

$$\begin{aligned} T^Z(\overline{\xi}) = &-(p_W)_* \left(\sum_k (-1)^k W_1 \bullet \operatorname{ch}(\operatorname{tr}_1(\overline{E})_k) \right) \\ &- \sum_k (-1)^k (p_P)_* [\widetilde{\operatorname{ch}}(\overline{\eta}_k)] + (p_P)_* (\operatorname{ch}(\pi_p^* \overline{F}) \operatorname{Td}^{-1}(\overline{Q}_1) \widetilde{e}_Z(\overline{Q}_1^\vee)). \end{aligned} \tag{9.33}$$

It follows directly from the definition that T^Z is the theory of singular Bott-Chern classes associated to the class

$$C_Z(F,N)=(p_P)_*(\operatorname{ch}(\pi_p^*\overline{F})\operatorname{Td}^{-1}(\overline{Q}_1)\widetilde{e}_Z(\overline{Q}_1^\vee)). \tag{9.34}$$

THEOREM 9.35. *The theory of singular Bott-Chern classes T^Z agrees with the theory of homogeneous singular Bott-Chern classes T^h.*

Proof. The result follows directly from theorem 7.1, equation (9.34) and proposition 9.18. □

Next we want to use 8.33 to give another characterization of T^h. To this end we only need to compute the characteristic class $C_{T^h}(\mathcal{O}_Y,L)$ for a line bundle L as a power series in $c_1(L)$.

THEOREM 9.36. *The theory of homogeneous singular Bott-Chern classes of algebraic vector bundles is the unique theory of singular Bott-Chern classes of algebraic vector bundles that is compatible with the projection formula and transitive and that satisfies*

$$C_{T^h}(\mathcal{O}_Y,L)=\mathbf{1}_1\bullet\phi(c_1(L)),$$

where ϕ is the power series

$$\phi(x)=\frac{1}{2}\sum_{n=0}^{\infty}\frac{(-1)^{n+1}H_{n+1}}{(n+2)!}x^n,$$

and where $H_n=1+\frac{1}{2}+\frac{1}{3}+\dots+\frac{1}{n}$, $n\geq 1$ are the harmonic numbers.

We already know that T^h is compatible with the projection formula and transitive. Thus it only remains to compute the power series ϕ.
Let $\overline{L}=(L,h_L)$ be a hermitian line bundle over a complex manifold Y. Let z be a system of holomorphic coordinates of Y. Let e be a local section of L and let $h(z)=h(e_z,e_z)$. Let $P=\mathbb{P}(L\oplus\mathbb{C})$, with $\pi\colon P\longrightarrow Y$ the projection and $\iota\colon Y\longrightarrow P$ the zero section. We choose homogeneous coordinates on P given by $(z,(x:y))$, here $(x:y)$ represents the line of $L_z\oplus\mathbb{C}$ generated by $xe(z)+y\mathbf{1}$, where $\mathbf{1}$ is a generator of $\mathbb{C}$ of norm 1. On the open set $y\neq 0$ we will use the absolute coordinate $t=x/y$. Let

$$0\longrightarrow\mathcal{O}(-1)\longrightarrow\pi^*(L\oplus\mathbb{C})\longrightarrow Q\longrightarrow 0$$

be the tautological exact sequence. The section $s=\{\mathbf{1}\}$ is a global section of Q that vanishes along the zero section. Moreover we have

$$\|s\|^2_{(z,(x:y))}=\frac{x\bar{x}h(z)}{y\bar{y}+x\bar{x}h(z)}=\frac{t\bar{t}h}{1+t\bar{t}h}.$$

Then (recall that we are using the algebro-geometric normalization)

$$c_1(\overline{Q}) = \partial\bar{\partial}\log\|s\|^2 \tag{9.37}$$
$$= \partial\bar{\partial}\log\frac{t\bar{t}h}{1+t\bar{t}h} \tag{9.38}$$
$$= \partial\left(\frac{1+t\bar{t}h}{t\bar{t}h}\frac{t\bar{\partial}(\bar{t}h)(1+t\bar{t}h)-t^2\bar{t}h\bar{\partial}(\bar{t}h)}{(1+t\bar{t}h)^2}\right) \tag{9.39}$$
$$= \partial\left(\frac{t\bar{\partial}(\bar{t}h)}{t\bar{t}h(1+t\bar{t}h)}\right) \tag{9.40}$$
$$= \partial\left(\frac{\bar{\partial}(\bar{t}h)}{\bar{t}h}\right)\frac{1}{1+t\bar{t}h} - \frac{\bar{t}\partial(ht)\wedge\bar{\partial}(\bar{t}h)}{\bar{t}h(1+t\bar{t}h)^2} \tag{9.41}$$
$$= \frac{\pi^*c_1(\overline{L})}{1+t\bar{t}h} - \frac{\partial(th)\wedge\bar{\partial}(\bar{t}h)}{h(1+t\bar{t}h)^2}. \tag{9.42}$$

We now consider the Koszul resolution

$$\overline{K}\colon 0 \longrightarrow Q^\vee \xrightarrow{s} \mathcal{O}_p \longrightarrow \iota_*\mathcal{O}_X \longrightarrow 0.$$

We denote by $T^h(\overline{K})$ the singular Bott-Chern class associated to this Koszul complex. Then, by proposition 9.13 and proposition 9.18,

$$T^h(\overline{K}) = -\frac{1}{2}\operatorname{Td}^{-1}(\overline{Q})\log\|s\|^2.$$

In order to compute $\pi_*T^h(\overline{K})$ we have to compute first $\pi_*c_1(\overline{Q})^n\log\|s\|^2$. But

$$c_1(\overline{Q})^n = \frac{\pi^*c_1(\overline{L})^n}{(1+t\bar{t}h)^n} - n\left(\frac{\pi^*c_1(\overline{L})}{(1+t\bar{t}h)}\right)^{n-1}\frac{\partial(th)\wedge\bar{\partial}(\bar{t}h)}{h(1+t\bar{t}h)^2}.$$

Therefore

$$\begin{aligned}\pi_*c_1(\overline{Q})^n\log\|s\|^2 &= -nc_1(\overline{L})^{n-1}\frac{1}{2\pi i}\int_{\mathbb{P}^1}\frac{\partial(th)\wedge\bar{\partial}(\bar{t}h)}{h(1+t\bar{t}h)^{n+1}}\log\frac{t\bar{t}h}{1+t\bar{t}h}\\ &= -nc_1(\overline{L})^{n-1}\frac{1}{2\pi i}\int_0^{2\pi}\int_0^\infty\log\frac{r^2}{1+r^2}\frac{-2ir\,\mathrm{d}\theta\,\mathrm{d}r}{(1+r^2)^{n+1}}\\ &= nc_1(\overline{L})^{n-1}\int_0^1\log(1-w)w^{n-1}\,\mathrm{d}w\\ &= -c_1(\overline{L})^{n-1}H_n,\end{aligned}$$

where H_n, $n\geq 1$ are the harmonic numbers. Since

$$Td^{-1}(\overline{Q}) = \frac{1-\exp(-c_1(\overline{Q}))}{c_1(\overline{Q})} = \sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!}c_1(\overline{Q})^n,$$

we obtain

$$C_{T^h}(\mathcal{O}_Y, L) = \pi_* T^h(\overline{K}) = \frac{1}{2}\sum_{n=0}^{\infty} \frac{(-1)^{n+1}H_{n+1}}{(n+2)!} c_1(\overline{L})^n \mathbf{1}_1.$$

Then, a reformulation of proposition 8.31 is

Corollary 9.43. *Let T be a theory of singular Bott-Chern classes for algebraic vector bundles that is compatible with the projection formula and transitive. Then there is a unique additive genus S_T such that*

$$C_T(F,N) - C_{T^h}(F,N) = \operatorname{ch}(F) \bullet \operatorname{Td}(N)^{-1} \bullet S_T(N). \tag{9.44}$$

Conversely, any additive genus determines a theory of singular Bott-Chern classes by the formula (9.44).

10 The arithmetic Riemann-Roch theorem for regular closed immersions

In this section we recall the definition of arithmetic Chow groups and arithmetic K-groups. We see that each choice of an additive theory of singular Bott-Chern classes allows us to define direct images for closed immersions in arithmetic K-theory. Once the direct images for closed immersions are defined, we prove the arithmetic Grothendieck-Riemann-Roch theorem for closed immersions. A version of this theorem was proved earlier by Bismut, Gillet and Soulé [6] when there is a commutative diagram

$$\begin{array}{ccc} \mathcal{Y} & \xrightarrow{\ i\ } & \mathcal{X} \\ & \searrow^{f} & \big\downarrow g \\ & & \mathcal{Z} \end{array},$$

where i is a closed immersion and f and g are smooth over $\mathbb{C}$. The version of this theorem given in this paper is due to Zha [32], but still unpublished. The theorem of Bismut, Gillet and Soulé compares $g_* \widehat{\operatorname{ch}}(i_*\overline{E})$ with $f_* \widehat{\operatorname{ch}}(\overline{E})$, whereas the theorem of Zha compares directly $\widehat{\operatorname{ch}}(i_*\overline{E})$ with $i_* \widehat{\operatorname{ch}}(\overline{E})$. The main difference between the theorem of Bismut, Gillet and Soulé and that of Zha is the kind of arithmetic Chow groups they use. In the first case these groups are only covariant for proper morphisms that are smooth over $\mathbb{C}$; thus the Grothendieck-Riemann-Roch can only be stated for a diagram as above, while in the second case a version of these groups that are covariant for arbitrary proper morphisms is used.

Since each choice of a theory of singular Bott-Chern classes gives rise to a different definition of direct images for closed immersions, the arithmetic Grothendieck-Riemann-Roch theorem will have a correction term that depends on the theory of singular Bott-Chern classes used. In the particular case of the

homogeneous singular Bott-Chern classes, which are the theories used by Bismut, Gillet and Soulé and by Zha, this correction term vanishes and we obtain the simplest formula. In this case the arithmetic Grothendieck-Riemann-Roch theorem is formally identical to the classical one.
Let (A, Σ, F_{∞}) be an arithmetic ring [18]. Since we will allow the arithmetic varieties to be non regular and we will use Chow groups indexed by dimension, following [20] we will assume that the ring A is equidimensional and Jacobson. Let F be the field of fractions of A. An *arithmetic variety* $\mathcal{X}$ is a scheme flat and quasi-projective over A such that $\mathcal{X}_F = \mathcal{X} \times \operatorname{Spec} F$ is smooth. Then $X := \mathcal{X}_{\Sigma}$ is a complex algebraic manifold, which is endowed with an anti-holomorphic automorphism F_{∞}. One also associates to $\mathcal{X}$ the real variety $X_{\mathbb{R}} = (X, F_{\infty})$.
Following [13], to each regular arithmetic variety we can associate different kinds of arithmetic Chow groups. Concerning arithmetic Chow groups, we shall use the terminology and notation in op. cit. §4 and §6.
Let $\mathcal{D}_{\log}$ be the Deligne complex of sheaves defined in [13] section 5.3; we refer to op. cit. for the precise definition and properties. A $\mathcal{D}_{\log}$-*arithmetic variety* is a pair $(\mathcal{X}, \mathcal{C})$ consisting of an arithmetic variety $\mathcal{X}$ and a complex of sheaves $\mathcal{C}$ on $X_{\mathbb{R}}$ which is a $\mathcal{D}_{\log}$-complex (see op. cit. section 3.1).
We are interested in the following $\mathcal{D}_{\log}$-complexes of sheaves:

(i) The Deligne complex $\mathcal{D}_{\mathrm{l,a},X}$ of differential forms on X with logarithmic and arbitrary singularities. That is, for every Zariski open subset U of X, we write

$$E^{*}_{\mathrm{l,a},X}(U) = \varinjlim_{\overline{U}} \Gamma(\overline{U}, \mathscr{E}^{*}_{\overline{U}}(\log B)),$$

where the limit is taken over all diagrams

$$\begin{array}{ccc} U & \xrightarrow{\overline{\iota}} & \overline{U} \\ & \searrow^{\iota} & \downarrow{\scriptstyle \beta} \\ & & X \end{array}$$

such that $\overline{\iota}$ is an open immersion, β is a proper morphism, $B = \overline{U} \setminus U$, is a normal crossing divisor and $\mathscr{E}^{*}_{\overline{U}}(\log B)$ denotes the sheaf of smooth differential forms on U with logarithmic singularities along B introduced in [8] .

For any Zariski open subset $U \subseteq X$, we put

$$\mathcal{D}^{*}_{\mathrm{l,a},X}(U,p) = (\mathcal{D}^{*}_{\mathrm{l,a},X}(U,p), \mathrm{d}_{\mathcal{D}}) = (\mathcal{D}^{*}(E_{\mathrm{l,a},X}(U), p), \mathrm{d}_{\mathcal{D}}).$$

If U is now a Zariski open subset of $X_{\mathbb{R}}$, then we write

$$\mathcal{D}^{*}_{\mathrm{l,a},X}(U,p) = (\mathcal{D}^{*}_{\mathrm{l,a},X}(U,p), \mathrm{d}_{\mathcal{D}}) = (\mathcal{D}^{*}_{\mathrm{l,a},X}(U_{\mathbb{C}},p)^{\sigma}, \mathrm{d}_{\mathcal{D}}),$$

where σ is the involution $\sigma(\eta) = \overline{F_{\infty}^{*}\eta}$ as in [13] notation 5.65.

Note that the sections of $\mathcal{D}^{*}_{\mathrm{l,a},X}$ over an open set $U \subset X$ are differential forms on U with logarithmic singularities along $X \setminus U$ and arbitrary singularities along $\overline{X} \setminus X$, where $\overline{X}$ is an arbitrary compactification of X. Therefore the complex of global sections satisfy

$$\mathcal{D}^{*}_{\mathrm{l,a},X}(X,*) = \mathcal{D}^{*}(X,*),$$

where the right hand side complex has been introduced in section §1. The complex $\mathcal{D}^{*}_{\mathrm{l,a},X}$ is a particular case of the construction of [12] section 3.6.

(ii) The Deligne complex $\mathcal{D}_{\mathrm{cur},X}$ of currents on X. This is the complex introduced in [13] definition 6.30.

When $\mathcal{X}$ is regular, applying the theory of [13] we can define the arithmetic Chow groups $\widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$ and $\widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$. These groups satisfy the following properties

(i) There are natural morphisms

$$\widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X}) \longrightarrow \widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$$

and, when applicable, all properties below will be compatible with these morphisms.

(ii) There is a product structure that turns $\widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})_{\mathbb{Q}}$ into an associative and commutative algebra. Moreover, it turns $\widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})_{\mathbb{Q}}$ into a $\widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})_{\mathbb{Q}}$-module.

(iii) If $f\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a map of regular arithmetic varieties, there are pull-back morphisms

$$f^{*}\colon \widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X}) \longrightarrow \widehat{\mathrm{CH}}^{*}(\mathcal{Y},\mathcal{D}_{\mathrm{l,a},Y}).$$

If moreover, f is smooth over F, there are pull-back morphisms

$$f^{*}\colon \widehat{\mathrm{CH}}^{*}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X}) \longrightarrow \widehat{\mathrm{CH}}^{*}(\mathcal{Y},\mathcal{D}_{\mathrm{cur},Y}).$$

The inverse image is compatible with the product structure.

(iv) If $f\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a proper map of regular arithmetic varieties of relative dimension d, there are push-forward morphisms

$$f_{*}\colon \widehat{\mathrm{CH}}^{*}(\mathcal{Y},\mathcal{D}_{\mathrm{cur},Y}) \longrightarrow \widehat{\mathrm{CH}}^{*-d}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X}).$$

If moreover, f is smooth over F, there are push-forward morphisms

$$f_{*}\colon \widehat{\mathrm{CH}}^{*}(\mathcal{Y},\mathcal{D}_{\mathrm{l,a},Y}) \longrightarrow \widehat{\mathrm{CH}}^{*-d}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X}).$$

The push-forward morphism satisfies the projection formula and is compatible with base change.

(v) The groups $\widehat{\mathrm{CH}}^*(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X})$ are naturally isomorphic to the groups defined by Gillet and Soulé in [18] (see [12] theorem 3.33). When X is generically projective, the groups $\widehat{\mathrm{CH}}^*(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X})$ are isomorphic to analogous groups introduced by Kawaguchi and Moriwaki [27] and are very similar to the weak arithmetic Chow groups introduced by Zha (see [11]).

(vi) There are well-defined maps

$$\begin{aligned} \zeta\colon\ & \widehat{\mathrm{CH}}^p(\mathcal{X}, \mathcal{C}) \longrightarrow \mathrm{CH}^p(\mathcal{X}), \\ \mathrm{a}\colon\ & \widetilde{\mathcal{C}}^{2p-1}(X_{\mathbb{R}}, p) \longrightarrow \widehat{\mathrm{CH}}^p(\mathcal{X}, \mathcal{C}), \\ \omega\colon\ & \widehat{\mathrm{CH}}^p(\mathcal{X}, \mathcal{C}) \longrightarrow \mathrm{Z}\mathcal{C}^{2p}(X_{\mathbb{R}}, p), \end{aligned}$$

where $\mathcal{C}$ is either $\mathcal{D}_{\mathrm{l,a},X}$ or $\mathcal{D}_{\mathrm{cur},X}$. For the precise definition of these maps see [13] notation 4.12.

When $\mathcal{X}$ is not necessarily regular, following [20] and combining with the definition of [13] we can define the arithmetic Chow groups indexed by dimension $\widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X})$ and $\widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X})$ (see [12] section 5.3).
They have the following properties (see [20]).

(i) If $\mathcal{X}$ is regular and equidimensional of dimension n then there are isomorphisms

$$\begin{aligned} \widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X}) &\cong \widehat{\mathrm{CH}}^{n-*}(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X}), \\ \widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X}) &\cong \widehat{\mathrm{CH}}^{n-*}(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X}). \end{aligned}$$

(ii) If $f\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a proper map between arithmetic varieties then there is a push-forward map

$$f_*\colon\ \widehat{\mathrm{CH}}_*(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y}) \longrightarrow \widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X}).$$

If f is smooth over F then there is a push-forward map

$$f_*\colon\ \widehat{\mathrm{CH}}_*(\mathcal{Y}, \mathcal{D}_{\mathrm{l,a},Y}) \longrightarrow \widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X}).$$

(iii) If $f\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a flat map or, more generally, a local complete intersection (l.c.i) map of relative dimension d, there are pull-back morphisms

$$f^*\colon\ \widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X}) \longrightarrow \widehat{\mathrm{CH}}_{*+d}(\mathcal{Y}, \mathcal{D}_{\mathrm{l,a},Y}).$$

If moreover, f is smooth over F, there are pull-back morphisms

$$f^*\colon\ \widehat{\mathrm{CH}}_*(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X}) \longrightarrow \widehat{\mathrm{CH}}_{*+d}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y}).$$

(iv) If $f\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a morphism of arithmetic varieties with $\mathcal{X}$ regular, then there is a cap product

$$\widehat{\mathrm{CH}}^{p}(\mathcal{X}, \mathcal{D}_{\mathrm{l,a},X}) \otimes \widehat{\mathrm{CH}}_{d}(\mathcal{Y}, \mathcal{D}_{\mathrm{l,a},Y}) \longrightarrow \widehat{\mathrm{CH}}_{d-p}(\mathcal{Y}, \mathcal{D}_{\mathrm{l,a},Y})_{\mathbb{Q}},$$

and a similar cap-product with the groups $\widehat{\mathrm{CH}}_{d}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y})$. This product is denoted by $y \otimes x \mapsto y._{f} x$,

For more properties of these groups see [20].
We will define now the arithmetic K-groups in this context. As a matter of convention, in the sequel we will use slanted letters to denote a object defined over A and the same letter in roman type for the corresponding object defined over $\mathbb{C}$. For instance we will denote a vector bundle over $\mathcal{X}$ by $\mathcal{E}$ and the corresponding vector bundle over X by E.

Definition 10.1. A *hermitian vector bundle* on an arithmetic variety $\mathcal{X}$, $\overline{\mathcal{E}}$, is a locally free sheaf $\mathcal{E}$ with a hermitian metric h_E on the vector bundle E induced on X, that is invariant under F_∞. A sequence of hermitian vector bundles on $\mathcal{X}$

$$(\overline{\varepsilon}) \qquad \dots \longrightarrow \overline{\mathcal{E}}_{n+1} \longrightarrow \overline{\mathcal{E}}_{n} \longrightarrow \overline{\mathcal{E}}_{n-1} \longrightarrow \dots$$

is said to be exact if it is exact as a sequence of vector bundles.
A *metrized coherent sheaf* is a pair $\overline{\mathcal{F}} = (\mathcal{F}, \overline{E}_* \to F)$, where $\mathcal{F}$ is a coherent sheaf on $\mathcal{X}$ and $\overline{E}_* \to F$ is a resolution of the coherent sheaf $F = \mathcal{F}_{\mathbb{C}}$ by hermitian vector bundles, that is defined over $\mathbb{R}$, hence is invariant under F_∞. We assume that the hermitian metrics are also invariant under F_∞.

Recall that to every hermitian vector bundle we can associate a collection of Chern forms, denoted by c_p. Moreover, the invariance of the hermitian metric under F_∞ implies that the Chern forms will be invariant under the involution σ. Thus

$$c_p(\overline{\mathcal{E}}) \in \mathcal{D}^{2p}_{\mathrm{l,a},X}(X_{\mathbb{R}}, p) = \mathcal{D}^{2p}(X, p)^{\sigma}.$$

We will denote also by $c_p(\overline{\mathcal{E}})$ its image in $\mathcal{D}^{2p}_{\mathrm{cur},X}(X_{\mathbb{R}}, p)$. In particular we have defined the Chern character $\mathrm{ch}(\overline{\mathcal{E}})$ in either of the groups $\bigoplus_p \mathcal{D}^{2p}_{\mathrm{l,a},X}(X_{\mathbb{R}}, p)$ or $\bigoplus_p \mathcal{D}^{2p}_{\mathrm{cur},X}(X_{\mathbb{R}}, p)$. Moreover, to each finite exact sequence $(\overline{\varepsilon})$ of hermitian vector bundles on $\mathcal{X}$ we can attach a secondary Bott-Chern class $\widetilde{\mathrm{ch}}(\overline{\varepsilon})$. Again, the fact that the sequence is defined over A and the invariance of the metrics with respect to F_∞ imply that

$$\widetilde{\mathrm{ch}}(\overline{\varepsilon}) \in \bigoplus_p \widetilde{\mathcal{D}}^{2p-1}_{\mathrm{l,a},X}(X_{\mathbb{R}}, p) = \bigoplus_p \widetilde{\mathcal{D}}^{2p-1}(X, p)^{\sigma}.$$

We will denote also by $\widetilde{\mathrm{ch}}(\overline{\varepsilon})$ its image in $\bigoplus_p \widetilde{\mathcal{D}}^{2p-1}_{\mathrm{cur},X}(X_{\mathbb{R}}, p)$. The Bott-Chern classes associated to exact sequences of metrized coherent sheaves enjoy the same properties.

Definition 10.2. Let $\mathcal{X}$ be an arithmetic variety and let $\mathcal{C}^*(*)$ be one of the two $\mathcal{D}_{\log}$-complexes $\mathcal{D}_{\mathrm{l,a},X}$ or $\mathcal{D}_{\mathrm{cur},X}$. The *arithmetic K-group* associated to the $\mathcal{D}_{\log}$-arithmetic variety $(\mathcal{X},\mathcal{C})$ is the abelian group $\widehat{K}(\mathcal{X},\mathcal{C})$ generated by pairs $(\overline{\mathcal{E}},\eta)$, where $\overline{\mathcal{E}}$ is a hermitian vector bundle on $\mathcal{X}$ and $\eta\in\bigoplus_{p\geq 0}\widetilde{\mathcal{C}}^{2p-1}(X_{\mathbb{R}},p)$, modulo relations

$$(\overline{\mathcal{E}}_1,\eta_1)+(\overline{\mathcal{E}}_2,\eta_2)=(\overline{\mathcal{E}},\tilde{\mathrm{ch}}(\overline{\varepsilon})+\eta_1+\eta_2) \tag{10.3}$$

for each short exact sequence

$$(\overline{\varepsilon})\qquad 0\longrightarrow\overline{\mathcal{E}}_1\longrightarrow\overline{\mathcal{E}}\longrightarrow\overline{\mathcal{E}}_2\longrightarrow 0\ .$$

The *arithmetic K'-group* associated to the $\mathcal{D}_{\log}$-arithmetic variety $(\mathcal{X},\mathcal{C})$ is the abelian group $\widehat{K}'(\mathcal{X},\mathcal{C})$ generated by pairs $(\overline{\mathcal{F}},\eta)$, where $\overline{\mathcal{F}}$ is a metrized coherent sheaf on $\mathcal{X}$ and $\eta\in\bigoplus_{p\geq 0}\widetilde{\mathcal{C}}^{2p-1}(X_{\mathbb{R}},p)$, modulo relations

$$(\overline{\mathcal{F}}_1,\eta_1)+(\overline{\mathcal{F}}_2,\eta_2)=(\overline{\mathcal{F}},\tilde{\mathrm{ch}}(\overline{\varepsilon})+\eta_1+\eta_2) \tag{10.4}$$

for each short exact sequence of metrized coherent sheaves

$$(\overline{\varepsilon})\qquad 0\longrightarrow\overline{\mathcal{F}}_1\longrightarrow\overline{\mathcal{F}}\longrightarrow\overline{\mathcal{F}}_2\longrightarrow 0\ .$$

We now give some properties of the arithmetic K-groups. As their proofs are similar, in the essential points, to those of analogous statements in, for example, [18] in the regular case and [20] in the singular case, we omit them.

(i) We have natural morphisms

$$\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})\longrightarrow\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})\text{ and }\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})\longrightarrow\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{cur},X}).$$

When applicable, all properties below will be compatible with these morphisms.

(ii) $\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$ is a ring. The product structure is given by

$$(\overline{\mathcal{F}}_1,\eta_1)\cdot(\overline{\mathcal{F}}_2,\eta_2)=(\overline{\mathcal{F}}_1\otimes\overline{\mathcal{F}}_2,\mathrm{ch}(\overline{\mathcal{F}}_1)\bullet\eta_2+\eta_1\bullet\mathrm{ch}(\overline{\mathcal{F}}_2)+\mathrm{d}_{\mathcal{D}}\,\eta_1\bullet\eta_2) \tag{10.5}$$

(iii) $\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$ is a $\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$-module.

(iv) There are natural maps

$$\widehat{K}(\mathcal{X},\mathcal{C})\longrightarrow\widehat{K}'(\mathcal{X},\mathcal{C})$$

that, when $\mathcal{X}$ is regular, are isomorphisms.

(v) The groups $\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$ and $\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$ are $\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$-modules.

(vi) There are natural maps

$$\omega\colon \widehat{K}'(\mathcal{X},\mathcal{C}) \longrightarrow \bigoplus_p Z\mathcal{C}^{2p}(p)$$

that send the class of a pair $(\overline{\mathcal{F}},\eta)$ with $\overline{\mathcal{F}}=(\mathcal{F},\overline{E}_*\to\mathcal{F}_{\mathbb{C}})$ to the form (or current)

$$\omega(\overline{\mathcal{F}},\eta)=\sum_i(-1)^i\operatorname{ch}(\overline{E}_i)+\mathrm{d}_{\mathcal{D}}\,\eta.$$

(vii) When $\mathcal{X}$ is regular, there exists a Chern character,

$$\widehat{\operatorname{ch}}\colon \widehat{K}(\mathcal{X},\mathcal{C})_{\mathbb{Q}} \longrightarrow \bigoplus_p \widehat{\operatorname{CH}}^p(\mathcal{X},\mathcal{C})_{\mathbb{Q}},$$

that is an isomorphism. Moreover, if $\mathcal{C}=\mathcal{D}_{\mathrm{l,a},X}$ this isomorphism is compatible with the product structure. If $\mathcal{X}$ is not regular, there is a biadditive pairing

$$\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})\otimes\widehat{\operatorname{CH}}_*(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})\longrightarrow\widehat{\operatorname{CH}}_*(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})_{\mathbb{Q}},$$

and a similar pairing with the groups $\widehat{\operatorname{CH}}_*(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$, which is denoted in both cases by $\alpha\otimes x\mapsto\widehat{\operatorname{ch}}(\alpha)\cap x$. For the properties of this product see [20] pg. 496.

(viii) If $\mathcal{Y}$ and $\mathcal{X}$ are arithmetic varieties and $f\colon\mathcal{Y}\to\mathcal{X}$ is a morphism of arithmetic varieties, f induces a morphism of rings:

$$f^*\colon \widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})\to\widehat{K}(\mathcal{Y},\mathcal{D}_{\mathrm{l,a},Y}).$$

When f is flat, the inverse image is also defined for the groups $\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$. Moreover, if $f_{\mathbb{C}}$ is smooth, the inverse image can be defined for the groups $\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$ and, when in addition f is flat, for the groups $\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$.

In what follows we will be interested in direct images for closed immersions. Since the direct images in arithmetic K-theory will depend on the choice of a metric, we have the following

Definition 10.6. A *metrized arithmetic variety* is a pair $(\mathcal{X},h_X)$ consisting of an arithmetic variety $\mathcal{X}$ and a hermitian metric on the complex tangent bundle T_X that is invariant under F_∞.

Let $(\mathcal{X},h_X)$ and $(\mathcal{Y},h_Y)$ be metrized arithmetic varieties and let $i\colon\mathcal{Y}\longrightarrow\mathcal{X}$ be a closed immersion. Over the complex numbers, we are in the situation of notation 8.36. In particular we have a canonical exact sequence of hermitian vector bundles

$$\overline{\xi}_N\colon 0\longrightarrow\overline{T}_Y\longrightarrow i^*\overline{T}_X\longrightarrow\overline{N}_{Y/X}\longrightarrow 0 \tag{10.7}$$

where the tangent bundles T_Y, T_X are endowed with the hermitian metrics h_Y, h_X respectively and the normal bundle $N_{Y/X}$ is endowed with an arbitrary hermitian metric h_N. We will follow the conventions of notation 8.36.
We next define push-forward maps, via a closed immersion, for the elements of the arithmetic K-group of a metrized arithmetic variety. We will define two kinds of push-forward maps. One will depend only on a metric on the complex normal bundle $N_{Y/X}$. By contrast, the second will depend on the choice of metrics on the complex tangent bundles T_X and T_Y. The second definition allows us to see $K'(\_, \mathcal{D}_{\mathrm{cur},Y})$ as a functor from the category whose objects are metrized arithmetic varieties and whose morphisms are closed immersions to the category of abelian groups.
As we deal with hermitian vector bundles and metrized coherent sheaves, both definitions will involve the choice of a theory of singular Bott-Chern classes. In order for the push forward to be well defined in K-theory we need a minimal additivity property for the singular Bott-Chern classes.

Definition 10.8. A theory of singular Bott-Chern classes T is called *additive* if for any closed embedding of complex manifolds $i\colon Y \hookrightarrow X$ and any hermitian embedded vector bundles $\overline{\xi}_1 = (i, \overline{N}, \overline{F}_1, \overline{E}_{1,*})$, $\overline{\xi}_2 = (i, \overline{N}, \overline{F}_2, \overline{E}_{2,*})$ the equation

$$T(\overline{\xi}_1 \oplus \overline{\xi}_2) = T(\overline{\xi}_1) + T(\overline{\xi}_2)$$

is satisfied.
Let C be a characteristic class for pairs of vector bundles. We say that it is *additive* (in the first variable) if

$$C(F_1 \oplus F_2, N) = C(F_1, N) + C(F_2, N)$$

for any vector bundles F_1, F_2, N on a complex manifold X.

The following statement follows directly from equation 7.5:

Proposition 10.9. *A theory of singular Bott-Chern classes T is additive if and only if the corresponding characteristic class C_T is additive in the first variable.*

Note that a theory of singular Bott-Chern classes consists in joining theories of singular Bott-Chern classes in arbitrary rank and codimension (definition 6.9). The property of being additive gives a compatibility condition for these theories, by respect to the hermitian vector bundles $\overline{F}$ (with the notation used in definition 6.9). Note also that if a theory of singular Bott-Chern classes is compatible with the projection formula then it is additive.

Definition 10.10. Let T be an additive theory of singular Bott-Chern classes, and let T_c be the associated covariant class as in definition 8.37. Let $i\colon (\mathcal{Y}, h_Y) \longrightarrow (\mathcal{X}, h_X)$ be a closed immersion of metrized arithmetic varieties and let $\overline{N} = \overline{N}_{Y/X} = (N_{Y/X}, h_N)$ be a choice of a hermitian metric on the complex normal bundle. The *push-forward maps*

$$i_*^{T_c}, i_*^{T}\colon \widehat{K}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y}) \longrightarrow \widehat{K}'(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X})$$

are defined by

$$\begin{aligned} i_*^{T_c}(\overline{\mathcal{F}},\eta) &= [((i_*\mathcal{F},\overline{E}_*\to(i_*\mathcal{F})_{\mathbb{C}}),0)]-[(0,T_c(\overline{\xi}_c))] \\ &\qquad +[(0,i_*(\eta\operatorname{Td}(Y)i^*\operatorname{Td}^{-1}(X)))] \qquad (10.11)\\ i_*^{T}(\overline{\mathcal{F}},\eta) &= [((i_*\mathcal{F},\overline{E}_*\to(i_*\mathcal{F})_{\mathbb{C}}),0)]-[(0,T(\overline{\xi}))] \\ &\qquad +[(0,i_*(\eta\operatorname{Td}^{-1}(\overline{N}_{Y/X})))]. \qquad (10.12)\end{aligned}$$

Here

$$0\to\overline{E}_n\to\dots\to\overline{E}_1\to\overline{E}_0\to(i_*\mathcal{F})_{\mathbb{C}}\to 0$$

is a finite resolution of the coherent sheaf $(i_*\mathcal{F})_{\mathbb{C}}$ by hermitian vector bundles, $\overline{\xi}=(i,\overline{N}_{X/Y},\overline{\mathcal{F}}_{\mathbb{C}},\overline{E}_*)$ is the induced hermitian embedded vector bundle on X, and $\overline{\xi}_c=(i,\overline{T}_X,\overline{T}_Y,\overline{\mathcal{F}}_{\mathbb{C}},\overline{E}_*)$ as in definition 8.37.
We can extend this definition to push-forward maps

$$i_*^{T_c},i_*^{T}\colon \widehat{K}'(\mathcal{Y},\mathcal{D}_{\mathrm{cur},Y})\longrightarrow\widehat{K}'(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$$

by the rule

$$\begin{aligned} i_*^{T_c}(\overline{\mathcal{F}},\eta) &= [((i_*\mathcal{F},\operatorname{Tot}(\overline{E}_{*,*})\to(i_*\mathcal{F})_{\mathbb{C}}),0)]-\sum_i(-1)^i[(0,T_c(\overline{\xi}_{i,c}))] \\ &\qquad +[(0,i_*(\eta\operatorname{Td}(Y)i^*\operatorname{Td}^{-1}(X)))], \qquad (10.13)\\ i_*^{T}(\overline{\mathcal{F}},\eta) &= [((i_*\mathcal{F},\operatorname{Tot}(\overline{E}_{*,*})\to(i_*\mathcal{F})_{\mathbb{C}}),0)]-\sum_i(-1)^i[(0,T(\overline{\xi}_i))] \\ &\qquad +[(0,i_*(\eta\operatorname{Td}^{-1}(\overline{N}_{Y/X})))], \qquad (10.14)\end{aligned}$$

where $0\to\overline{E}_n\to\dots\to\overline{E}_0\to\mathcal{F}_{\mathbb{C}}\to 0$ is a resolution of $\mathcal{F}_{\mathbb{C}}$ by hermitian vector bundles, $\overline{E}_{*,*}$ is a complex of complexes of vector bundles over X, such that, for each $i\geq 0$, $\overline{E}_{i,*}\to i_*E_i$ is also a resolution by hermitian vector bundles and $\overline{\xi}_i=(i,\overline{N}_{X/Y},\overline{E}_i,\overline{E}_{i,*})$ is the induced hermitian embedded vector bundle and $\overline{\xi}_{i,c}$ is as in definition 8.37. We suppose that there is a commutative diagram of resolutions

$$\begin{array}{ccccccccc} \cdots & \longrightarrow & E_{k+1,*} & \longrightarrow & E_{k,*} & \longrightarrow & E_{k-1,*} & \longrightarrow & \cdots.\\ & & \downarrow & & \downarrow & & \downarrow & & \\ \cdots & \longrightarrow & i_*E_{k+1} & \longrightarrow & i_*E_k & \longrightarrow & i_*E_{k-1} & \longrightarrow & \cdots \end{array}$$

hence a resolution $\operatorname{Tot}(\overline{E}_{*,*})\longrightarrow(i_*\mathcal{F})_{\mathbb{C}}$ by hermitian vector bundles.

Note that, whenever the push-forward i_*^T appears, we will assume that we have chosen a metric on $N_{Y/X}$.
The two push-forward maps are related by the equation

$$i_*^{T_c}(\overline{\mathcal{F}},\eta)=i_*^{T}(\overline{\mathcal{F}},\eta)-\left[\left(0,i_*\left(\omega(\overline{\mathcal{F}},\eta)\widetilde{\operatorname{Td}^{-1}}(\overline{\xi}_N)\operatorname{Td}(Y)\right)\right)\right], \qquad (10.15)$$

where $\overline{\xi}_N$ is the exact sequence (10.7).

Proposition 10.16. *The push-forward maps i_*^T, $i_*^{T_c}$ are well defined. That is, they do not depend on the choice of a representative of a class in $\widehat{K}$, nor on the choice of metrics on the coherent sheaf $(i_*\mathcal{F})_{\mathbb{C}}$. The first one does not depend on the choice of metrics on T_X nor on T_Y, whereas the second one does not depend on the choice of a metric on the normal bundle $N_{Y/X}$. Moreover, if i is a regular closed immersion or $\mathcal{X}$ is a regular arithmetic variety, then $i_*^{T_c}$ and i_*^T can be lifted to maps*

$$i_*^{T_c}, i_*^T\colon \widehat{K}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y}) \longrightarrow \widehat{K}(\mathcal{X}, \mathcal{D}_{\mathrm{cur},Y}).$$

Proof. The fact that i_*^T only depends on the metric on $\overline{N}$ and not on the metrics on T_X and T_Y and that for $i_*^{T_c}$ is the opposite, follows directly from the definition in the first case and from proposition 8.39 in the second.
We will only prove the other statements for $i_*^{T_c}$, as the other case is analogous. We first prove the independence from the metric chosen on the coherent sheaf $(i_*\mathcal{F})_{\mathbb{C}}$. If $\overline{E}_* \to (i_*\mathcal{F})_{\mathbb{C}}$, $\overline{E}'_* \to (i_*\mathcal{F})_{\mathbb{C}}$ are two such metrics, inducing the hermitian embedded vector bundles $\overline{\xi}$ respectively $\overline{\xi}'$, then, using corollary 6.14

$$T_c(\overline{\xi}'_c) - T_c(\overline{\xi}_c) = T(\overline{\xi}') - T(\overline{\xi}) = \widetilde{\mathrm{ch}}(\overline{\varepsilon}),$$

where $\overline{\varepsilon}$ is the exact complex of hermitian embedded vector bundles

$$\overline{\varepsilon}\colon 0 \longrightarrow \overline{\xi} \longrightarrow \overline{\xi}' \longrightarrow 0,$$

where $\overline{\xi}'$ sits in degree zero.
Therefore, by equation 10.4,

$$\begin{aligned}&[((i_*\mathcal{F}, \overline{E}_* \to (i_*\mathcal{F})_{\mathbb{C}}), 0)] - [(0, T_c(\overline{\xi_c}))]\\ &\qquad\qquad = [((i_*\mathcal{F}, \overline{E}'_* \to (i_*\mathcal{F})_{\mathbb{C}}), 0)] - [(0, T_c(\overline{\xi}'_c))].\end{aligned}$$

Since the last term of equation 10.11 does not depend on the metric on $(i_*\mathcal{F})_{\mathbb{C}}$, we obtain that $i_*^{T_c}$ does not depend on this metric.
For proving that the push-forward map $i_*^{T_c}$ is well defined it remains to show the independence from the choice of a representative of a class in $\widehat{K}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y})$. We consider an exact sequence of hermitian vector bundles on $\mathcal{Y}$

$$\overline{\varepsilon}\colon 0 \longrightarrow \overline{\mathcal{F}}_1 \longrightarrow \overline{\mathcal{F}} \longrightarrow \overline{\mathcal{F}}_2 \longrightarrow 0$$

and two classes $\eta_1, \eta_2 \in \bigoplus_{p\geq 0} \widetilde{\mathcal{D}}^{2p-1}_{\mathrm{cur}}(Y, p)$. We also denote $\overline{\varepsilon}$ the induced exact sequence of hermitian vector bundles on Y. We have to prove

$$i_*^{T_c}([(\overline{\mathcal{F}}, \eta_1 + \eta_2 + \widetilde{\mathrm{ch}}(\overline{\varepsilon})]) = i_*^{T_c}([(\overline{\mathcal{F}_1}, \eta_1)]) + i_*^{T_c}([(\overline{\mathcal{F}_2}, \eta_2)]). \tag{10.17}$$

Since it is clear that $i_*^{T_c}(0, \eta_1 + \eta_2) = i_*^{T_c}(0, \eta_1) + i_*^{T_c}(0, \eta_2)$, we are led to prove

$$i_*^{T_c}([(\overline{\mathcal{F}}, \widetilde{\mathrm{ch}}(\overline{\varepsilon})]) = i_*^{T_c}([(\overline{\mathcal{F}_1}, 0)]) + i_*^{T_c}([(\overline{\mathcal{F}_2}, 0)]). \tag{10.18}$$

We choose metrics on the coherent sheaves $(i_*\mathcal{F}_1)_{\mathbb{C}}$, $(i_*\mathcal{F}_2)_{\mathbb{C}}$ and $(i_*\mathcal{F})_{\mathbb{C}}$ respectively:

$$\overline{E}_{1,*} \longrightarrow (i_*\mathcal{F}_1)_{\mathbb{C}}\ ,\ \overline{E}_{2,*} \longrightarrow (i_*\mathcal{F}_2)_{\mathbb{C}}\ ,\ \overline{E}_{*} \longrightarrow (i_*\mathcal{F})_{\mathbb{C}}.$$

We denote $\overline{\xi}_1$, $\overline{\xi}_2$, $\overline{\xi}$ the induced hermitian embedded vector bundles. We obtain an exact sequence of metrized coherent sheaves on $\mathcal{X}$:

$$\overline{\nu}\colon 0 \longrightarrow \overline{i_*\mathcal{F}_1} \longrightarrow \overline{i_*\mathcal{F}} \longrightarrow \overline{i_*\mathcal{F}_2} \longrightarrow 0.$$

Then, using the fact that the theory T is additive and equation (8.42) we have

$$T_c(\overline{\xi}_{1,c}) + T_c(\overline{\xi}_{2,c}) - T_c(\overline{\xi}_c) = [\widetilde{\operatorname{ch}}(\overline{\nu})] - i_*([\widetilde{\operatorname{ch}}(\overline{\varepsilon}) \bullet \operatorname{Td}(Y)]) \bullet \operatorname{Td}^{-1}(X). \quad (10.19)$$

Moreover, by the relation (10.4),

$$[(\overline{i_*\mathcal{F}_1}, 0)] + [(\overline{i_*\mathcal{F}_2}, 0)] = [(\overline{i_*\mathcal{F}}, \widetilde{\operatorname{ch}}(\overline{\nu}))]. \quad (10.20)$$

Hence, we compute,

$$\begin{aligned}
i_*^{T_c}([(\overline{\mathcal{F}}, \widetilde{\operatorname{ch}}(\overline{\varepsilon})]) &- i_*^{T_c}([(\overline{\mathcal{F}_1}, 0)]) - i_*^{T_c}([(\overline{\mathcal{F}_2}, 0)]) \\
&= [(i_*\overline{\mathcal{F}}, 0)] - [(i_*\overline{\mathcal{F}_1}, 0)] - [(i_*\overline{\mathcal{F}_2}, 0)] \\
&\quad - [(0, T_c(\overline{\xi}_c))] + [(0, T_c(\overline{\xi_{1,c}}))] + [(0, T_c(\overline{\xi_{2,c}}))] \\
&\quad + [(0, i_*([\widetilde{\operatorname{ch}}(\overline{\varepsilon})] \bullet \operatorname{Td}(Y) \bullet i^* \operatorname{Td}^{-1}(X)))] \\
&= -[(0, i_*([\widetilde{\operatorname{ch}}(\overline{\varepsilon})] \bullet \operatorname{Td}(Y) \bullet i^* \operatorname{Td}^{-1}(X))))] \\
&\quad + [(0, i_*([\widetilde{\operatorname{ch}}(\overline{\varepsilon})] \bullet \operatorname{Td}(Y) \bullet i^* \operatorname{Td}^{-1}(X))))] \\
&= 0.
\end{aligned}$$

The proof that $i_*^{T_c}$ for metrized coherent sheaves is well defined is similar. The proof of its independence from choice of a metric on $N_{Y/X}$ or from the choice of the resolutions and metrics in X is the same as before. Now let

$$0 \longrightarrow \overline{\mathcal{F}}' \longrightarrow \overline{\mathcal{F}} \longrightarrow \overline{\mathcal{F}}'' \longrightarrow 0$$

be a short exact sequence of metrized coherent sheaves on $\mathcal{Y}$. This means that we have resolutions $\overline{E}'_* \to \mathcal{F}'_{\mathbb{C}}$, $\overline{E}_* \to \mathcal{F}_{\mathbb{C}}$ and $\overline{E}''_* \to \mathcal{F}''_{\mathbb{C}}$. Using theorem 2.24 we can suppose that there is a commutative diagram of resolutions

$$\begin{array}{ccccccccc}
0 & \to & \overline{E}'_* & \to & \overline{E}_* & \to & \overline{E}''_* & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & \mathcal{F}'_{\mathbb{C}} & \to & \mathcal{F}_{\mathbb{C}} & \to & \mathcal{F}''_{\mathbb{C}} & \to & 0,
\end{array} \quad (10.21)$$

with exact rows. Moreover, we can assume that the complexes of complexes $\overline{E}'_{*,*}$, $\overline{E}_{*,*}$, $\overline{E}''_{*,*}$ used in definition 10.10 are chosen compatible with diagram (10.21). Thus we obtain a commutative diagram

$$\begin{array}{ccccccccc}
0 & \to & \operatorname{Tot}\overline{E}'_{*,*} & \to & \operatorname{Tot}\overline{E}_{*,*} & \to & \operatorname{Tot}\overline{E}''_{*,*} & \to & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \to & i_*\mathcal{F}'_{\mathbb{C}} & \to & i_*\mathcal{F}_{\mathbb{C}} & \to & i_*\mathcal{F}''_{\mathbb{C}} & \to & 0.
\end{array} \quad (10.22)$$

We denote by $\overline{\nu}$ the exact sequence of metrized coherent sheaves on X defined by diagram (10.22). We denote $\overline{\chi}_i$ the exact sequence of hermitian vector bundles on Y

$$\overline{\chi}_i\colon 0 \longrightarrow \overline{E}'_i \longrightarrow \overline{E}_i \longrightarrow \overline{E}''_i \longrightarrow 0,$$

and by $\overline{\varepsilon}$ the exact sequence of metrized coherent sheaves on X

$$\overline{\varepsilon}_i\colon 0 \longrightarrow \overline{i_*E}'_i \longrightarrow \overline{i_*E_i} \longrightarrow \overline{i_*E}''_i \longrightarrow 0.$$

Moreover, let $\overline{\xi}_i$, $\overline{\xi}'_i$ and $\overline{\xi}''_i$ denote the hermitian embedded vector bundles defined by the above resolutions and $\overline{E}_i$, $\overline{E}'_i$ and $\overline{E}''_i$ respectively and let $\overline{\xi}_{i,c}$, $\overline{\xi}'_{i,c}$ and $\overline{\xi}''_{i,c}$ be as in definition 8.37. Then, using proposition 2.38 and equation (8.42) we obtain

$$\begin{aligned}\widetilde{\mathrm{ch}}(\overline{\nu}) &= \sum_i (-1)^i \widetilde{\mathrm{ch}}(\overline{\varepsilon}) \\ &= \sum_i (-1)^i (T_c(\overline{\xi}'_{i,c}) + T_c(\overline{\xi}''_{i,c}) - T_c(\overline{\xi}_{i,c})) \\ &\quad + \sum_i (-1)^i i_*(\widetilde{\mathrm{ch}}(\overline{\chi}_i) \bullet \mathrm{Td}(Y)) \bullet \mathrm{Td}^{-1}(X)\end{aligned} \tag{10.23}$$

Now the proof follows as before, but using equation (10.23) instead of equation (10.19).

If $\mathcal{X}$ is a regular arithmetic variety, the lifting property follows from the isomorphism between the $\widehat{K}$-groups and the $\widehat{K}'$-groups.

Suppose now that $i\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a regular closed immersion and let $[\overline{\mathcal{F}}, \eta] \in \widehat{K}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y})$. Then it follows from [2] III that the coherent sheaf $i_*\mathcal{F}$ can be resolved

$$0 \longrightarrow \mathcal{E}_n \longrightarrow \dots \longrightarrow \mathcal{E}_0 \longrightarrow i_*\mathcal{F} \longrightarrow 0$$

with $\mathcal{E}_i$ locally free sheaves on $\mathcal{X}$. Moreover we endow the vector bundles E_i induced on X with hermitian metrics and so we obtain a metric on the coherent sheaf $i_*\mathcal{F}$ and the corresponding hermitian embedded vector bundle $\overline{\xi}$. Using the independence from the resolutions and on the metrics we see that the equation 10.11 defines an element in $\widehat{K}(\mathcal{X}, \mathcal{D}_{\mathrm{cur},X})$. □

Proposition 10.24. *For any element $\alpha \in \widehat{K}'(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y})$ we have*

$$\omega(i_*^{T_c}(\alpha))\,\mathrm{Td}(X) = i_*(\omega(\alpha)\,\mathrm{Td}(Y)) \tag{10.25}$$

$$\omega(i_*^{T}(\alpha)) = i_*(\omega(\alpha)\,\mathrm{Td}^{-1}(N_{Y/X})) \tag{10.26}$$

Proof. We will prove the statement only for $i_*^{T_c}$. We consider first a class of the form $[\overline{\mathcal{F}}, 0]$. Using equation (8.38) we obtain, after choosing a metric $\overline{E}_i \longrightarrow (i_*\mathcal{F})_{\mathbb{C}}$, and considering the induced hermitian embedded vector bundle

$\overline{\xi_c}$:

$$\begin{aligned}\omega(i_*^{T_c}([\overline{\mathcal{F}},0]))\operatorname{Td}(X) &= \Big(\sum(-1)^i\operatorname{ch}(\overline{E_i}) - \mathrm{d}_{\mathcal{D}}\, T_c(\overline{\xi_c})\Big)\operatorname{Td}(X)\\ &= i_*(\operatorname{ch}(\overline{F})\bullet\operatorname{Td}(Y)\bullet i^*\operatorname{Td}^{-1}(X)i^*(\operatorname{Td}(X)))\\ &= i_*(\operatorname{ch}(\overline{F})\bullet\operatorname{Td}(Y))\\ &= i_*(\omega([\overline{\mathcal{F}},0])\operatorname{Td}(Y))\end{aligned}$$

Taking now a class of the form $[0,\eta]$ we obtain:

$$\begin{aligned}\omega(i_*^{T_c}([0,\eta]))\operatorname{Td}(X) &= \mathrm{d}_{\mathcal{D}}\left(i_*(\eta\operatorname{Td}(Y)i^*\operatorname{Td}^{-1}(X))\right)\operatorname{Td}(X)\\ &= i_*\,\mathrm{d}_{\mathcal{D}}(\eta\operatorname{Td}(Y))\\ &= i_*(\omega([0,\eta])\operatorname{Td}(Y))\end{aligned}$$

and hence the equality 10.25 is proved. □

The next proposition explains the terminology "compatible with the projection formula" and "transitive" that we used for theories of singular Bott-Chern classes. The second statement is the main reason to introduce the push-forward $i_*^{T_c}$.

Proposition 10.27. *If the theory of singular Bott-Chern classes is compatible with the projection formula, we have that, for $\alpha\in\widehat{K}'(\mathcal{Y},\mathcal{D}_{\mathrm{cur},Y})$ and $\beta\in\widehat{K}(\mathcal{X},\mathcal{D}_{\mathrm{l,a},X})$ the following equalities hold*

$$\begin{aligned}i_*^{T_c}(\alpha i^*\beta) &= i_*^{T_c}(\alpha)\beta,\\ i_*^{T}(\alpha i^*\beta) &= i_*^{T}(\alpha)\beta.\end{aligned}$$

If moreover the theory of singular Bott-Chern classes is transitive and $j\colon(\mathcal{Z},h_Z)\longrightarrow(\mathcal{Y},h_Y)$ is another closed immersion of metrized arithmetic varieties, then

$$(i\circ j)_*^{T_c} = i_*^{T_c}\circ j_*^{T_c}.$$

Proof. We prove first the projection formula. For simplicity we will treat the case when $\alpha\in\widehat{K}(\mathcal{Y},\mathcal{D}_{\mathrm{cur},Y})$. Let $\alpha=(\overline{\mathcal{F}},\eta)$, let $\overline{\xi_c}=(i,\overline{T}_X,\overline{T}_Y,\overline{\mathcal{F}}_{\mathbb{C}},\overline{E}_*)$ be a hermitian embedded vector bundle and let $\beta=(\overline{\mathcal{E}},\chi)$. Using equations (10.11) and (10.5), we obtain

$$\begin{aligned}i_*^{T_c}(\alpha i^*\beta) - i_*^{T_c}(\alpha)\beta &= -\sum_i(-1)^i\operatorname{ch}(\overline{E}_i)\bullet\chi + \mathrm{d}_{\mathcal{D}}(T_c(\overline{\xi}_c))\bullet\chi\\ &\quad + i_*(\operatorname{ch}((\overline{\mathcal{F}})_{\mathbb{C}})\bullet\operatorname{Td}(Y)))\bullet\operatorname{Td}^{-1}(X)\bullet\chi\\ &\quad + T_c(\overline{\xi}_c)\bullet\operatorname{ch}(\overline{\mathcal{E}}_{\mathbb{C}}) - T_c(\overline{\xi}_c\otimes\overline{\mathcal{E}}_{\mathbb{C}})\\ &= T_c(\overline{\xi}_c\otimes\overline{\mathcal{E}}_{\mathbb{C}}) - T_c(\overline{\xi}_c)\bullet\operatorname{ch}(\overline{\mathcal{E}}_{\mathbb{C}}).\end{aligned}$$

Therefore, if T is compatible with the projection formula, then the projection formula holds.

The fact that, if moreover T is transitive then $(i\circ j)_*^{T_c}=i_*^{T_c}\circ j_*^{T_c}$ follows directly from the definition and equation (8.41). □

If $i\colon \mathcal{Y} \longrightarrow \mathcal{X}$ is a regular closed immersion between arithmetic varieties, then the normal cone $\mathcal{N}_{\mathcal{Y}/\mathcal{X}}$ is a locally free sheaf. The choice of a hermitian metric on $N_{Y/X}$ determines a hermitian vector bundle $\overline{\mathcal{N}}_{\mathcal{Y}/\mathcal{X}}$. If now $i\colon (\mathcal{Y}, h_Y) \longrightarrow (\mathcal{X}, h_X)$ is a closed immersion between regular metrized arithmetic varieties, then the tangent bundles $\mathcal{T}_{\mathcal{Y}}$ and $\mathcal{T}_{\mathcal{X}}$ are virtual vector bundles. Since over $\mathbb{C}$ they define vector bundles, we can provide them with hermitian metrics and denote the hermitian virtual vector bundles by $\overline{\mathcal{T}}_{\mathcal{X}}$ and $\overline{\mathcal{T}}_{\mathcal{Y}}$. There are well defined clases $\widehat{\mathrm{Td}}(\mathcal{Y}) = \widehat{\mathrm{Td}}(\overline{\mathcal{T}}_{\mathcal{Y}})$ and $\widehat{\mathrm{Td}}(\mathcal{X}) = \widehat{\mathrm{Td}}(\overline{\mathcal{T}}_{\mathcal{X}})$.
The arithmetic Grothendieck-Riemann-Roch theorem for closed immersions compares the direct images in the arithmetic K-groups with the direct images in the arithmetic Chow groups.

Theorem 10.28 ([6], [32]). *Let T be a theory of singular Bott-Chern classes and let S_T be the additive genus of corollary 9.43.*

(i) Let $i\colon \mathcal{Y} \longrightarrow \mathcal{X}$ be a regular closed immersion between arithmetic varieties. Assume that we have chosen a hermitian metric on the complex bundle $N_{Y/X}$. Then, for any $\alpha = (\overline{\mathcal{F}}, \eta) \in \widehat{K}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y})$ the equation

$$\widehat{\mathrm{ch}}(i_*^T(\alpha)) = i_*(\widehat{\mathrm{ch}}(\alpha)\widehat{\mathrm{Td}}^{-1}(\overline{\mathcal{N}}_{\mathcal{Y}/\mathcal{X}})) - \mathrm{a}(i_*(\mathrm{ch}(\mathcal{F}_{\mathbb{C}})\,\mathrm{Td}^{-1}(N_{Y/X})S_T(N)) \tag{10.29}$$

holds.

(ii) Let $i\colon (\mathcal{Y}, h_Y) \longrightarrow (\mathcal{X}, h_X)$ be a closed immersion between regular metrized arithmetic varieties. Then, for any $\alpha = (\overline{\mathcal{F}}, \eta) \in \widehat{K}(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y})$ the equation

$$\widehat{\mathrm{ch}}(i_*^{T_c}(\alpha))\widehat{\mathrm{Td}}(\mathcal{X}) = i_*(\widehat{\mathrm{ch}}(\alpha)\widehat{\mathrm{Td}}(\mathcal{Y})) - \mathrm{a}(i_*(\mathrm{ch}(\mathcal{F}_{\mathbb{C}})\,\mathrm{Td}(Y)S_T(N))) \tag{10.30}$$

holds.

Proof. The proof follows the classical pattern of the deformation to the normal cone as in [6] and [32].
Let $\mathcal{W}$ be the deformation to the normal cone to $\mathcal{Y}$ in $\mathcal{X}$. We will follow the notation of section 5. Since i is a regular closed immersion, there is a finite resolution by locally free sheaves

$$0 \to \mathcal{E}_n \to \cdots \to \mathcal{E}_1 \to \mathcal{E}_0 \to i_*\mathcal{F} \to 0.$$

We choose hermitian metrics on the complex bundles $E_i = (\mathcal{E}_i)_{\mathbb{C}}$. The immersion $j\colon \mathcal{Y} \times \mathbb{P}^1 \longrightarrow \mathcal{W}$ is also a regular immersion. The construction of theorem 5.4 is valid over the arithmetic ring A. Therefore we have a resolution by hermitian vector bundles

$$0 \to \widetilde{\mathcal{G}}_n \to \cdots \to \widetilde{\mathcal{G}}_1 \to \widetilde{\mathcal{G}}_0 \to i_*\mathcal{F} \to 0.$$

such that its restriction to $\mathcal{X}\times\{0\}$ is isometric to $\mathcal{E}_*$. Its restriction to $\widetilde{\mathcal{X}}$ is orthogonally split, and its restriction to $\mathcal{P}=\mathbb{P}(\mathcal{N}_{\mathcal{Y}/\mathcal{X}}\oplus\mathcal{O}_{\mathcal{Y}})$ fits in a short exact sequence

$$0\longrightarrow\overline{\mathcal{A}}_*\longrightarrow\widetilde{\mathcal{E}}_*|_{\mathcal{P}}\longrightarrow K(\overline{\mathcal{F}},\overline{\mathcal{N}}_{\mathcal{Y}/\mathcal{X}})\longrightarrow 0,$$

where $\overline{\mathcal{A}}_*$ is orthogonally split and $K(\overline{\mathcal{F}},\overline{\mathcal{N}}_{\mathcal{Y}/\mathcal{X}})$ is the Koszul resolution. We denote by $\overline{\eta}_k$ the piece of degree k of this exact sequence. Let t be the absolute coordinate of $\mathbb{P}^1$. It defines a rational function in $\mathcal{W}$ and

$$\widehat{\operatorname{div}}(t)=(\mathcal{X}_0+\mathcal{P}+\widetilde{\mathcal{X}},(0,-\frac{1}{2}\log t\bar{t}))$$

The key point of the proof of the theorem is that, in the group $\widehat{\mathrm{CH}}^*(\mathcal{X},\mathcal{D}_{\mathrm{cur},X})$, we have

$$(p_{\mathcal{W}})_*(\widehat{\mathrm{ch}}(\widetilde{\mathcal{E}}_*)\widehat{\operatorname{div}}(t))=0.$$

Using the definition of the product in the arithmetic Chow rings we obtain

$$(p_{\mathcal{W}})_*(\widehat{\mathrm{ch}}(\widetilde{\mathcal{E}}_*)\widehat{\operatorname{div}}(t))=\widehat{\mathrm{ch}}(\overline{\mathcal{E}}_*)-(p_{\widetilde{\mathcal{X}}})_*\widehat{\mathrm{ch}}(\widetilde{\mathcal{E}}_*|_{\widetilde{\mathcal{X}}})-(p_{\widetilde{\mathcal{P}}})_*\widehat{\mathrm{ch}}(\widetilde{\mathcal{E}}_*|_{\mathcal{P}})\\+\mathrm{a}((p_W)_*(\mathrm{ch}((\widetilde{\mathcal{E}}_*)_{\mathbb{C}})\bullet W_1)).\tag{10.31}$$

But we have

$$\widehat{\mathrm{ch}}(\overline{\mathcal{E}}_*)=\widehat{\mathrm{ch}}(i_*^T(\overline{\mathcal{F}}))+\mathrm{a}(T(\overline{\xi})),\tag{10.32}$$

$$(p_{\widetilde{\mathcal{X}}})_*\widehat{\mathrm{ch}}(\widetilde{\mathcal{E}}_*|_{\widetilde{\mathcal{X}}})=0,\tag{10.33}$$

$$(p_{\widetilde{\mathcal{P}}})_*\widehat{\mathrm{ch}}(\widetilde{\mathcal{E}}_*|_{\mathcal{P}})=i_*(\pi_{\mathcal{P}})_*(\widehat{\mathrm{ch}}(K(\overline{\mathcal{F}},\overline{\mathcal{N}}_{\mathcal{Y}/\mathcal{X}}))-\sum_k(-1)^k\,\mathrm{a}(\widetilde{\mathrm{ch}}(\overline{\eta}_k))).\tag{10.34}$$

Moreover, by equation (7.3),

$$\mathrm{a}((p_W)_*(\mathrm{ch}((\widetilde{\mathcal{E}}_*)_{\mathbb{C}})\bullet W_1))=-\,\mathrm{a}(T(\overline{\xi}))-\sum_k(-1)^k\,\mathrm{a}(\widetilde{\mathrm{ch}}(\overline{\eta}_k)))\\+\mathrm{a}(i_*C_T(\mathcal{F}_{\mathbb{C}},\mathcal{N}_{\mathbb{C}})).\tag{10.35}$$

Thus we are led to compute $i_*(\pi_{\mathcal{P}})_*\widehat{\mathrm{ch}}(K(\overline{\mathcal{F}},\overline{\mathcal{N}}_{\mathcal{Y}/\mathcal{X}}))$. This is done in the following two lemmas.

Lemma 10.36. *Let $\mathcal{Y}$ be an arithmetic variety, $\overline{\mathcal{N}}$ a rank r hermitian vector bundle over $\mathcal{Y}$ and denote $\mathcal{P}=\mathbb{P}^1(\mathcal{N}\oplus\mathcal{O}_{\mathcal{Y}})$, and $\overline{\mathcal{Q}}$ the tautological quotient bundle. Let $\mathcal{Y}_0$ be the cycle defined by the zero section of $\mathcal{P}$. Then*

$$\widehat{c}_r(\overline{\mathcal{Q}})=(\mathcal{Y}_0,(c_r(\overline{\mathcal{Q}}_{\mathbb{C}}),\widetilde{e}(\mathcal{P}_{\mathbb{C}},\overline{\mathcal{Q}}_{\mathbb{C}},s))),\tag{10.37}$$

where $\widetilde{e}(\mathcal{P}_{\mathbb{C}},\overline{\mathcal{Q}}_{\mathbb{C}},s)$ is the Euler-Green current of lemma 9.4.

Proof. We know that $\widehat{c}_r(\overline{\mathcal{Q}}) = (\mathcal{Y}_0, (c_r(\overline{\mathcal{Q}}_{\mathbb{C}}), \widetilde{e}))$ for certain Green current $\widetilde{e}$. By definition this Green current satisfies

$$\mathrm{d}_{\mathcal{D}} \widetilde{e} = c_r(\overline{\mathcal{Q}}_{\mathbb{C}}) - \delta_{\mathcal{Y}_{\mathbb{C}}}.$$

Moreover, since the restriction of $\overline{\mathcal{Q}}_{\mathbb{C}}$ to D_∞ has a global section of constant norm we have that $\widetilde{e}|_{D_\infty} = 0$. Therefore, by lemma 9.4,

$$\widetilde{e} = \widetilde{e}(\mathcal{P}_{\mathbb{C}}, \overline{\mathcal{Q}}_{\mathbb{C}}, s).$$

□

Lemma 10.38. *The following equality hold:*

$$(\pi_{\mathcal{P}})_*\widehat{\mathrm{ch}}(K(\overline{\mathcal{F}},\overline{\mathcal{N}})_*) = \widehat{\mathrm{ch}}(\overline{\mathcal{F}})\widehat{\mathrm{Td}^{-1}}(\overline{\mathcal{N}}) + \mathrm{a}(C_T(\overline{\mathcal{F}},\overline{\mathcal{N}}) - \mathrm{ch}(\mathcal{F}_{\mathbb{C}})\,\mathrm{Td}^{-1}(N_{Y/X})S_T(N)). \tag{10.39}$$

Proof. We just compute, using lemma 10.36,

$$\begin{aligned}
(\pi_{\mathcal{P}})_*\widehat{\mathrm{ch}}(K(\overline{\mathcal{F}},\overline{\mathcal{N}})_*) &= (\pi_{\mathcal{P}})_* \sum_k (-1)^k \widehat{\mathrm{ch}}(\bigwedge^k \overline{\mathcal{Q}}^\vee)\widehat{\mathrm{ch}}(\pi_{\mathcal{P}}^*\overline{\mathcal{F}}) \\
&= (\pi_{\mathcal{P}})_*(\widehat{c}_r(\overline{\mathcal{Q}})\widehat{\mathrm{Td}^{-1}}(\overline{\mathcal{Q}}))\widehat{\mathrm{ch}}(\overline{\mathcal{F}}) \\
&= \widehat{\mathrm{Td}^{-1}}(\overline{\mathcal{N}})\widehat{\mathrm{ch}}(\overline{\mathcal{F}}) + \mathrm{a}((\pi_P)_*(\widetilde{e}\,\mathrm{Td}^{-1}(\overline{Q}))\,\mathrm{ch}(\overline{F})) \\
&= \widehat{\mathrm{Td}^{-1}}(\overline{\mathcal{N}})\widehat{\mathrm{ch}}(\overline{\mathcal{F}}) + \mathrm{a}((\pi_P)_*(T^h(K(\overline{F},\overline{N})))\,\mathrm{ch}(\overline{F})) \\
&= \widehat{\mathrm{Td}^{-1}}(\overline{\mathcal{N}})\widehat{\mathrm{ch}}(\overline{\mathcal{F}}) + \mathrm{a}(C_{T^h}(F,N)) \\
&= \widehat{\mathrm{Td}^{-1}}(\overline{\mathcal{N}})\widehat{\mathrm{ch}}(\overline{\mathcal{F}}) + C_T(F,N) - \mathrm{a}(\mathrm{Td}^{-1}(N)\,\mathrm{ch}(F)S_T(N)).
\end{aligned}$$

□

The equation (10.29) follows by combining equations (10.31), (10.32), (10.33), (10.34), (10.35) and (10.39).
The equation (10.30) follows from equation (10.29) by a straightforward computation. □

Since T is homogeneous if and only if $S_T = 0$, in view of this result, the theory of homogeneous singular Bott-Chern classes is characterized for being the unique theory of singular Bott-Chern classes that provides an exact arithmetic Grothendieck-Riemann-Roch theorem for closed immersions. By contrast, if one uses a theory of singular Bott-Chern classes that is not homogeneous, there is an analogy between the genus S_T and the R-genus that appears in the arithmetic Grothendieck-Riemann-Roch theorem for submersions.
Since there is a unique theory of homogeneous singular Bott-Chern classes, the following definition is natural.

Definition 10.40. Let $i\colon (\mathcal{Y}, h_Y) \longrightarrow (\mathcal{X}, h_X)$ be a closed immersion of metrized arithmetic varieties, the *push-forward map*

$$i_*\colon \widehat{K}'(\mathcal{Y}, \mathcal{D}_{\mathrm{cur},Y}) \longrightarrow \widehat{K}'(\mathcal{X}, \mathcal{D}_{\mathrm{cur},Y})$$

is defined as $i_* = i_*^{T_c^h}$.

Corollary 10.41. *The push-forward map makes* $\widehat{K}'(\_, \mathcal{D}_{\mathrm{cur},Y})$ *and* $\widehat{K}(\_, \mathcal{D}_{\mathrm{cur},Y})$ *functors from the category of regular metrized arithmetic varieties and closed immersions to the category of abelian groups.*

Corollary 10.42. *Let* $i\colon (\mathcal{Y}, h_Y) \longrightarrow (\mathcal{X}, h_X)$ *be a closed immersion of regular metrized arithmetic varieties, then*

$$\widehat{\mathrm{ch}}(i_*^T(\alpha))\widehat{\mathrm{Td}}(\mathcal{X}) = i_*(\widehat{\mathrm{ch}}(\alpha)\widehat{\mathrm{Td}}(\mathcal{Y})). \tag{10.43}$$

Remark 10.44. Combining theorem 10.28 with [16] we can obtain an arithmetic Grothendieck-Riemann-Roch theorem for projective morphisms of regular arithmetic varieties.
In a forthcoming paper we will show that the higher torsion forms used to define the direct images for submersions can also be characterized axiomatically.

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Hicas of Length ≤ 4

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Abstract. A *hica* is a highest weight, homogeneous, indecomposable, Calabi-Yau category of dimension 0. A hica has length l if its objects have Loewy length l and smaller. We classify hicas of length ≤ 4, up to equivalence, and study their properties. Over a fixed field F, we prove that hicas of length 4 are in one-one correspondence with bipartite graphs. We prove that an algebra A_Γ controlling the hica associated to a bipartite graph Γ is Koszul, if and only if Γ is not a simply laced Dynkin graph, if and only if the quadratic dual of A_Γ is Calabi-Yau of dimension 3.

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1. Introduction

Once a mathematical definition has been made, the theory surrounding that definition usually begins with a study of small examples. A striking violation of this principle occurred at the birth of category theory, where early theory was concerned with establishing results valid for large and floppy mathematical structures like the category of sets, or the category of groups, or the category of topological spaces. But time has passed, categories have begun to be taken seriously, and they are now objects of detailed study. Since categories are often large and floppy, the 2-category of all categories is very large and very floppy. To prove theorems about categories, it is necessary to make strong restrictions on their structure. To prove classification theorems for categories, it is necessary to make very strong restrictions on their structure.

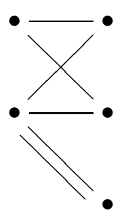
There is by now an extensive collection of categorical classification theorems. A category with one object and invertible morphisms is a group, and there are many examples of classification theorems in group theory. Rings are endowed with various categories, like their module categories. Classification theorems for commutative rings can be thought of as classification theorems in algebraic geometry. There are a number of classification theorems for rings of finite

homological dimension, to which the term noncommutative geometry is applied. For example, hereditary algebras over an algebraically closed field can be parametrised by quivers. Calabi-Yau algebras of dimensions 2 and 3 can be loosely parametrised by quivers with a superpotential [2], [5], [8]. Categorical classification theorems also appear in the representation theory of 2-categories: irreducible integrable representations of 2-Kac-Moody Lie algebras can be parametrised by integral dominant weights [18].
Our paper runs in this vein. A *hica* is a highest weight, homogeneous, indecomposable, Calabi-Yau category of dimension 0. Here, we say a highest weight category is homogeneous if its standard objects all have the same Loewy length, and its costandard objects all have the same Loewy length. We say a hica has length l if its projective objects have Loewy length l and smaller. We classify hicas of length ≤ 4 up to equivalence.
Hicas show up naturally in group representation theory and in the theory of tilings [20, 3, 14, 15]. A multitude of examples of hicas were constructed by Mazorchuk and Miemietz [13]. Every hica can be realised as the module category of some symmetric quasi-hereditary algebra. If the hica is not semisimple, the corresponding algebra is necessarily infinite dimensional, noncommutative, of infinite homological dimension.
Let us fix a field F, and consider hicas over F, up to equivalence. The only hica of length 1 is the category of vector spaces over F. There are no hicas of length 2. There is a unique hica of length 3, which is the module category of the Brauer tree algebra on a bi-infinite line. Our first main result is

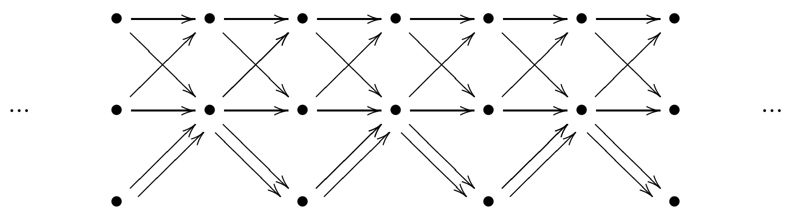
Theorem 1. *There is a natural one-one correspondence*

$$\{\textit{bipartite graphs}\} \leftrightarrow \{\textit{hicas of length } 4\}.$$

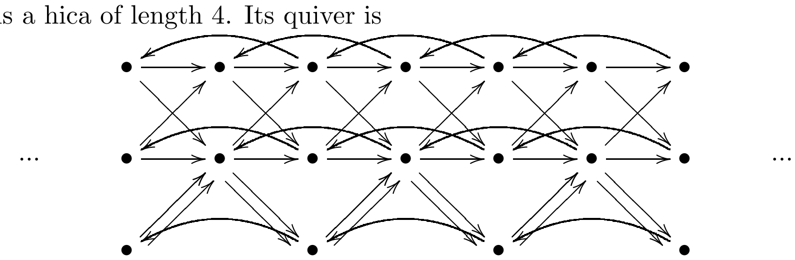
Here, and throughout this paper, a bipartite graph will by definition be connected.
The one-one correspondence of Theorem 1 is obtained from a sequence of three one-one correspondences: a one-one correspondence between bipartite graphs and topsy-turvy quivers; a one-one correspondence between topsy-turvy quivers and basic indecomposable self-injective directed algebras of Loewy length 3; and a one-one correspondence between basic self-injective directed algebras of Loewy length 3 and hicas of length 4.
Let us describe here the construction of a hica $\mathcal{C}_\Gamma$ of length 4 from the following bipartite graph Γ:



First, we construct a quiver Q_Γ, by consecutively gluing together opposite orientations of this bipartite graph, one next to the other:



This quiver has an automorphism ϕ which shifts a vertex to a vertex which is two steps horizontally to its right. We take the path algebra of this quiver. We now construct a self-injective directed algebra B_Γ of Loewy length 3, factoring the path algebra by relations which insist that all squares commute, and that paths $u \to v \to w$ of length 2 are zero, unless $w = \phi(u)$. We define A_Γ to be the trivial extension $B_\Gamma \oplus B_\Gamma^*$ of B_Γ by its dual. The module category $\mathcal{C}_\Gamma$ of A_Γ is a hica of length 4. Its quiver is



The relations for A_Γ are those for B_Γ, along with relations which insist that the product of two leftwards pointing arrows is zero whilst squares involving a pair of parallel leftwards pointing arrows commute. The algebra A_Γ has some pleasing properties. It admits a derived self-equivalence ψ_γ for every vertex γ of Γ. It also admits a number of $\mathbb{Z}_+^3$-gradings, one for each orientation of the graph Γ. It is Koszul and its quadratic dual $A_\Gamma^!$ is Calabi-Yau of dimension 3. More generally, we have the following theorem.

Theorem 2. *Suppose* Γ *is a connected bipartite graph, and* $\mathcal{C}_\Gamma = A_\Gamma$-mod *the associated hica of length* 4. *The following are equivalent:*

1. Γ *is not a simply laced Dynkin graph.*
2. A_Γ *is Koszul.*
3. *The quadratic dual of* A_Γ *is Calabi-Yau of dimension* 3.

The way this paper evolved was surprising to us. We began with the problem of classifying small hicas, categories whose structural features (Calabi-Yau 0, highest weight) were motivated by exposure to group representation theory. We ended having made contact with mathematics of different kin: bipartite graphs, Calabi-Yau 3s, and Dynkin classifications. The hica restrictions indeed capture some features of Lie theoretic representation theory, but they can also be thought of as noncommutative geometric restrictions: highest weight categories were invented to capture stratification properties appearing in algebraic geometry, whilst 0-Calabi-Yau categories are categories possessing a homological duality with trivial Serre functor.

2. Preliminaries

Our main objects of study, *hicas*, are a species of abelian categories. As we study them, we will use freely the languages of abelian categories, algebras, and triangulated categories. Here we give a short phrasebook for these languages.
Let F be a field. The collection of F-algebras is a 2-category, whose arrows are bimodules ${}_AM_B$ which are flat on the right, and 2-arrows are bimodule homomorphisms. We have a 2-functor

$$\mathfrak{Algebra} \to \mathfrak{Abelian}$$

from the 2-category $\mathfrak{Algebra}$ of F-algebras to the 2-category $\mathfrak{Abelian}$ of abelian categories. This 2-functor takes an algebra A to its module category, a bimodule ${}_AM_B$ to the functor $M \otimes_B -$, and a bimodule homomorphism to a natural transformation. We have a 2-functor

$$\mathfrak{Abelian} \to \mathfrak{Triangulated}$$

taking values in the 2-category of triangulated categories, which takes an abelian category $\mathcal{A}$ to its derived category $D(\mathcal{A})$.
If X is an object of an abelian category of finite composition length, we define the *Loewy length* of X (or *length* of X, or $l(X)$) to be the smallest number l for which there exists a filtration of X with l nonzero sections, all of which are semisimple. We define the *head*, or *top* of X to be the maximal semisimple quotient of X, and the *socle* of X to be the maximal semisimple submodule.
If $\mathcal{A}$ is an abelian category, we define the *length* of $\mathcal{A}$ to be the supremum over all lengths of objects in $\mathcal{A}$. If A is an algebra, we define the *length* of A to be the length of the abelian category A-mod of A-modules.
Given a finite dimensional F-vector space V, we denote by V^* the dual $Hom_F(V,F)$ of V. We call an object X of a triangulated category *compact* if $\mathrm{Hom}(X,-)$ commutes with infinite direct sums. We say an F-linear triangulated category $\mathcal{T}$ is *Calabi-Yau of dimension* d if $\mathrm{Hom}_{\mathcal{T}}(P,X)$ is finite dimensional for objects $X \in \mathcal{T}$, and compact objects $P \in \mathcal{T}$, and

$$\mathrm{Hom}_{\mathcal{T}}(P,X) \cong \mathrm{Hom}_{\mathcal{T}}(X,P[d])^*$$

naturally in objects $X \in \mathcal{T}$, and compact objects $P \in \mathcal{T}$. For background, we recommend a survey article of B. Keller concerning Calabi-Yau triangulated categories [8]. To avoid confusion here, let us emphasise that the definition of a Calabi-Yau triangulated category Keller uses is slightly different from this one since he makes no compactness assumption on P.
We say an F-linear abelian category $\mathcal{A}$ is Calabi-Yau of dimension d if its derived category $D(\mathcal{A})$ is Calabi-Yau of dimension d. We say an F-algebra A is Calabi-Yau of dimension d if its module category A-mod is Calabi-Yau of dimension d.

Suppose A is a basic (not necessarily unital) F-algebra satisfying the following assumptions:

(i) A has a countable set $\{e_x \mid x \in \Lambda\}$ of orthogonal primitive idempotents, such that $A = \oplus_{x,y} e_x A e_y$;
(ii) for any $x, y \in \Lambda$ the F-vector space $e_x A e_y$ is finite dimensional;
(iii) for any $x \in \Lambda$ there exist only finitely many $y \in \Lambda$ such that $e_x A e_y \neq 0$;
(iv) for any $x \in \Lambda$ there exist only finitely many $y \in \Lambda$ such that $e_y A e_x \neq 0$.

Under these assumptions all indecomposable projective A-modules Ae_x and all injective A-modules $\mathrm{Hom}_F(e_x A, F)$ are finite-dimensional. A-modules $M = {}_A M$ will be left A-modules unless they carry a right subscript as in M_A in which case they will be right A-modules. We denote by A-mod the collection of all finite-dimensional left A-modules and by mod-A the collection of all finite-dimensional right A-modules. We denote by A-perf the subcategory of the derived category of A-mod consisting of perfect complexes, that is the smallest thick subcategory of the derived category of A-mod containing all projective objects of A-mod, or equivalently the subcategory of compact objects in the derived category of A. We define A^* to be the A-A-bimodule $\bigoplus_{x\in\Lambda} \mathrm{Hom}_F(Ae_x, F)$.
We say A is a *symmetric algebra* if $A \cong A^*$ as A-A-bimodules. Then A is symmetric if and only if A-mod is Calabi-Yau of dimension 0 (cf. [17], Theorem 3.1).
Suppose A is an algebra satisfying the above conditions, and Λ is ordered. For $\lambda \in \Lambda$, let $J_{\geq\lambda} = \sum_{\mu\geq\lambda} Ae_\mu A$ and $J_{>\lambda} = \sum_{\mu>\lambda} Ae_\mu A$. Let $J_\lambda = J_{\geq\lambda}/J_{>\lambda}$. We say A is *quasi-hereditary* if the product map $J_\lambda e_\lambda \otimes_F e_\lambda J_\lambda \to J_\lambda$ is an isomorphism for every $\lambda \in \Lambda$ [4].

Now suppose $\mathcal{A}$ is an abelian category over F, with enough projective objects, enough injective objects, and a countable set Λ indexing the isomorphism classes of simple objects of $\mathcal{A}$, such that all objects of $\mathcal{A}$ have a finite composition series with sections in Λ. Abusing notation, an element λ of Λ we sometimes take to represent an index, sometimes an isomorphism class of irreducible object, and sometimes a representative of the latter. We denote by $P(\lambda)$ a minimal projective cover of λ in $\mathcal{A}$. Such exist, since we have enough projectives, and finite composition series.
We call $\mathcal{A}$ a *highest weight category* [4] if there is an ordering $<$ on Λ, and a collection of objects $\Delta(\lambda)$, for $\lambda \in \Lambda$, such that

(i) there is an epimorphism $\Delta(\lambda) \twoheadrightarrow \lambda$ whose kernel $X(\lambda)$ has composition factors $\mu < \lambda$;
(ii) $P(\lambda)$ has a filtration with a single section isomorphic to $\Delta(\lambda)$ and every other section isomorphic to $\Delta(\mu)$, for $\mu > \lambda$.

If A is quasi-hereditary, then A-mod is a highest weight category, with standard objects ${}_A\Delta(\lambda) = J_\lambda e_\lambda$, and mod-$A$ is a highest weight category with standard modules $\Delta_A(\lambda) = e_\lambda J_\lambda$. Thus A has a filtration by ideals, whose sections are

isomorphic to
$$_A\Delta(\lambda) \otimes_F \Delta_A(\lambda).$$
Conversely, if $\mathcal{A}$ is a highest weight category, then $A = \oplus_{\lambda,\mu\in\Lambda} Hom(P(\lambda), P(\mu))$ is a quasi-hereditary algebra.
The left and right costandard modules $_A\nabla(\lambda)$, $\nabla(\lambda)_A$ of A are defined to be the duals of the right and left standard modules $\nabla(\lambda)_A$, $_A\nabla(\lambda)$ of A. We write $\Delta = \oplus_\lambda \Delta(\lambda)$ and $\nabla = \oplus_\lambda \nabla(\lambda)$.

Lemma 3. *Let A be a selfinjective quasi-hereditary algebra. If A is not semisimple, then A is infinite dimensional.*

Proof. Nonsemisimple selfinjective algebras have infinite homological dimension, since Heller translation is invertible. Finite dimensional quasi-hereditary algebras have finite homological dimension. □

We say a highest weight category $\mathcal{C}$ is homogeneous if its standard objects all have the same Loewy length, and its costandard objects all have the same Loewy length. Equivalently, $\mathcal{C} = A$-mod, where A is a quasi-hereditary algebra whose left standard modules all have the same Loewy length, and whose right standard modules all have the same Loewy length.

Definition 4. *A* hica *is is a <u>hi</u>ghest weight, <u>h</u>omogeneous, <u>i</u>ndecomposable <u>Ca</u>labi-Yau <u>ca</u>tegory of dimension* 0*.*

The collection $\mathfrak{Hica}$ of hicas forms a 2-category (arrows are exact functors, 2-arrows are natural transformations). We denote by $\mathfrak{Hica}_l$ the 2-category of hicas of length l.

Lemma 5. *The* 2*-functor*
$$\{\textit{symmetric, homogeneous, quasihereditary basic algebras }\} \twoheadrightarrow \mathfrak{Hica}$$
which takes an algebra to its module category is essentially bijective on objects.

Proof. We must define a correspondence between objects of our 2-categories, under which isomorphic algebras correspond to equivalent categories, and vice versa. If A is a symmetric, Δ-homogeneous quasihereditary algebra then A-mod is a hica ([4], [17], Theorem 3.1). If $\mathcal{C}$ is a hica, then $A = \oplus_{\lambda\in\Lambda} \mathrm{Hom}(P(\lambda), P(\mu))$ is an algebra such that A-mod $= \mathcal{C}$. □

A highest weight category $\mathcal{C}$ has a collection of indecomposable tilting modules $T(\lambda)$ indexed by Λ, characterised as indecomposable objects with a Δ-filtration and a ∇-filtration. The *Ringel dual* $\mathcal{C}'$ of $\mathcal{C}$ is the module category A'-mod of the algebra
$$A' = \oplus_{\lambda,\mu} \mathrm{Hom}_{\mathcal{C}}(T(\lambda), T(\mu)).$$
The Ringel dual $\mathcal{C}'$ of $\mathcal{C}$ is a highest weight category. If $\mathcal{C} = A$-mod, we call A' the Ringel dual of A. If $\mathcal{C} \cong \mathcal{C}'$ then we say $\mathcal{C}$ and A are *Ringel self-dual.*

Lemma 6. *Suppose $\mathcal{C} = A$-mod is a hica. Then*
$$l(A) = l(_A\Delta) + l(\Delta_A) - 1.$$

Proof. The length of A is the least number l such that the product of any l elements of the radical of A is zero. This can be otherwise defined as the radical length of the $A \otimes A^{op}$-module A. Since A is quasi-hereditary, ${}_AA_A$ has a bimodule filtration with sections ${}_A\Delta(\lambda) \otimes_F \Delta_A(\lambda)$. These sections have radical length $l({}_A\Delta) + l(\Delta_A) - 1$, as $A \otimes A^{op}$-modules. Therefore the Loewy length of A is at least $l({}_A\Delta) + l(\Delta_A) - 1$.
The tops of all of these sections lie in the top of ${}_AA_A$. Since A is symmetric, every irreducible lies in the socle of A. Since A is also quasi-hereditary, every irreducible lies in the socle of some standard object Δ. Given $\lambda \in \Lambda$, the socle Fx_λ of Ae_λ is generated by $\mathrm{soc}({}_A\Delta(\nu)) \otimes_F \mathrm{soc}(\Delta_A(\nu))$, for suitable ν, modulo lower terms in the filtration. The lower terms in the filtration have zero intersection with Fx_λ, since this space is one dimensional. Therefore, lifting an element of $\mathrm{soc}({}_A\Delta(\nu)) \otimes \mathrm{soc}(\Delta_A(\nu))$ to an element of radical length $l({}_A\Delta) + l(\Delta_A) - 1$ in A, we obtain an element of Fx_λ of radical length $l({}_A\Delta) + l(\Delta_A) - 1$. It follows that the Loewy length of A is at most $l({}_A\Delta) + l(\Delta_A) - 1$. □

We also wish to consider graded algebras, which may satisfy weaker assumptions than those given above. If G is a group, and A an algebra, then a G-grading of A is a decomposition $A = \oplus_{g \in G} A^g$, such that $A^g.A^h \subset A^{gh}$. A graded A-module is an A module with a decomposition $M = \oplus_{g \in G} M^g$, such that $A^g.M^h \subset M^{gh}$; a homomorphism $\phi : M \to N$ of graded modules is an A-module homomorphism sending M^g to N^g, for $g \in G$.
We say A is $\mathbb{Z}_+$-graded if it is $\mathbb{Z}$-graded, with $A^i = 0$ for $i < 0$. Suppose A a $\mathbb{Z}$-graded algebra, whose degree 0 part A^0 satisfies the conditions (i)-(iv) above. Then we denote by A-mod the abelian subcategory of the category of all A-modules generated by A^0-mod, and by A-gr the abelian subcategory of the category of all graded A-modules generated by the category of finite dimensional A^0-mod$\langle i \rangle$, for $i \in \mathbb{Z}$. We denote by A-grperf the thick subcategory of the the derived category of graded A-modules generated by objects of the form $A \otimes_{A^0} X\langle i \rangle$, where $X \in A^0$-mod and $i \in \mathbb{Z}$.

3. Elementary constructions

Let us give some elementary constructions of symmetric algebras.
Suppose B is an algebra. Let $A = T(B)$ denote the trivial extension of B by B^*. Then A is symmetric, and A-mod is Calabi-Yau of dimension 0.
Suppose B is an algebra and M is a B-B-bimodule such that $e_\lambda M e_\mu$ is finite-dimensional for every $\lambda, \mu \in \Lambda$ and such that for every λ only finitely many of $e_\lambda M e_\mu$ and $e_\mu M e_\lambda$ are non-zero. Define $M^* := \bigoplus_{\lambda \in \Lambda} \mathrm{Hom}_F(Me_\lambda, F)$ and assume we have a fixed bimodule isomorphism $M \cong M^*$. Then we have a

sequence of bimodule homomorphisms

$$\begin{aligned}B \to \mathrm{Hom}_B(M,M) \cong \mathrm{Hom}_B(M,M^*) &= \mathrm{Hom}_B(M, \bigoplus_{\lambda\in\Lambda} \mathrm{Hom}(Me_\lambda, F))\\ &\cong \bigoplus_{\lambda\in\Lambda} \mathrm{Hom}_B(M, \mathrm{Hom}(Me_\lambda, F))\\ &\cong \bigoplus_{\lambda\in\Lambda} \mathrm{Hom}_F(M\otimes_B Me_\lambda, F)\\ &= \bigoplus_{\lambda\in\Lambda} \mathrm{Hom}_F((M\otimes_B M)e_\lambda, F)\\ &= (M\otimes_B M)^*,\end{aligned}$$

noting that $M \otimes_B M$ satisfies that $e_\lambda M \otimes_B Me_\mu = \bigoplus_{\nu\in\Lambda} e_\lambda Me_\nu \otimes_B e_\nu Me_\mu$ is finite-dimensional (finitely many finite-dimensional direct summands) for all λ, μ, and for every λ only finitely many of $e_\lambda M \otimes_B Me_\mu$ and $e_\mu M \otimes_B Me_\lambda$ are nonzero. The obtained bimodule homomorphisms compose to give a bimodule homomorphism $B \to (M \otimes_B M)^*$. Let $\mu : M \otimes_B M \to B^*$ denote the dual map.

Associated to the data (B, M), we have a $\mathbb{Z}$-graded algebra $U = U(B, M)$ concentrated in degrees 0,1, and 2 whose degree 0,1,2 part is B,M, B^* respectively. The product map $U^0 \otimes U^i \to U^i$ is given by the left action of B on the bimodule U^i, for $i = 0, 1, 2$. The product map $U^i \otimes U^0 \to U^i$ is given by the right action of B on the bimodule U^i. We define the product $U^1 \otimes_{U^0} U^1 \to U^2$ to be given by μ. The product is associative since the product of three components $U^i \otimes U^j \otimes U^k$ is non-zero if and only if $i + j + k \leq 2$, in which case associativity is clearly visible.

Lemma 7. *$U(B, M)$-mod is Calabi-Yau of dimension zero.*

Proof. We have a bimodule isomorphism $U \cong U^*$ which exchanges U^0 and U^2, and sends U^1 to U^{1*} via the fixed isomorphism $M \cong M^*$. □

4. Topsy-turvy quivers

Given a vertex w in a quiver Q, let $\mathcal{P}(w)$ denote the collection of vertices v of Q for which there is an arrow pointing from v to w (the *past* of w), counted with multiplicity. Let $\mathcal{F}(u)$ denote the collection of vertices v of Q for which there is an arrow pointing from u to v (the *future* of u), counted with multiplicity.

Definition 8. *A connected quiver is* topsy-turvy *if it contains at least one arrow, and there is an automorphism ϕ of the vertices of Q such that $\mathcal{F}(u) = \mathcal{P}(u^\phi)$ for every vertex u of Q.*

For any topsy-turvy quiver, the automorphism ϕ extends to a quiver automorphism, since arrows from x to y can be placed in bijection with arrows from y to x^ϕ, which can be placed in bijection with arrows from x^ϕ to y^ϕ.

Lemma 9. *If Q is a topsy-turvy quiver, then $\mathcal{PF}(w) = \mathcal{FP}(w)$ for all vertices w of Q.*

Proof. Any x in $\mathcal{FP}(w)$ lies in the future of some u in the past of w, and therefore lies in the past of u^ϕ; since Q is topsy-turvy, u^ϕ also lies in the future of w and x lies in $\mathcal{PF}(w)$. By symmetry, if x lies in $\mathcal{PF}(w)$ then x also lies in $\mathcal{FP}(w)$. □

A directed topsy-turvy quiver Q can be $\mathbb{Z}$-graded in the following way: take an arbitrary vertex u of Q and place it in degree 0. We say another vertex v in Q is in degree k if there exist $i_1, \ldots, i_r$ and $j_1, \ldots, j_r$ such that $v \in \mathcal{P}^{i_1}\mathcal{F}^{j_1} \ldots \mathcal{P}^{i_r}\mathcal{F}^{j_r}(u)$ and $\sum_{1 \leq s \leq r} j_s - \sum_{1 \leq s \leq r} i_s = k$. This is well-defined since $\mathcal{PF}(w) = \mathcal{FP}(w)$. It follows that all arrows in Q point from degree i to degree $i+1$ and that ϕ has degree 2.
A *bipartite graph* is a countable connected graph Γ whose set V of vertices decomposes into two nonempty subsets $V = V_l \cup \Gamma_r$ such that no edges of Γ connect V_l to V_l, or V_r to V_r. Note that we do *not* call the graph with one vertex and no arrows bipartite.
Given a graph Γ with a bipartite decomposition of vertices $V = V_l \cup V_r$, we have an associated directed topsy-turvy quiver Q_Γ, obtained by orienting $\mathbb{Z}$ copies of Γ, identifying, for i even, the r-vertices of i^{th} copy of Γ with the r-vertices of the $i+1^{th}$ copy of Γ, the l-vertices of i^{th} copy of Γ with the l-vertices of the $i-1^{th}$ copy of Γ, and insisting that arrows in the i^{th} copy of Γ point from the $i-1^{th}$ copy to the $i+1^{th}$ copy, for $i \in \mathbb{Z}$. Note that if we label our bipartite decomposition with the opposite orientation, we obtain an isomorphic topsy-turvy quiver.

Lemma 10. *We have a one-one correspondence $\Gamma \leftrightarrow Q_\Gamma$ between bipartite graphs and directed topsy-turvy quivers.*

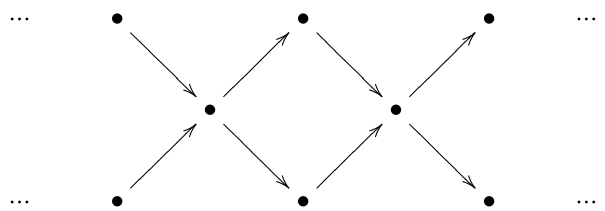
Proof. Given a directed topsy-turvy quiver, we have a $\mathbb{Z}$-grading of the set of vertices $V = \amalg_{i \in \mathbb{Z}} V_i$, see above. Let A_i denote the set of arrows from V_i to V_{i+1}. The set of arrows of our quiver is graded $A = \amalg_{i \in \mathbb{Z}} A_i$. The automorphism ϕ defines isomorphisms between V_i and V_j and between A_i and A_j when i and j are both even, or when i and j are both odd. We can thus identify the V_i for i even with a single vertex set V_{even}, the V_i for i odd with a single vertex set V_{odd}, the A_i for i even with a single arrow set A_{eo} from V_{even} to V_{odd}, the A_i for i odd with a single arrow set A_{oe} from V_{odd} to V_{even}. The topsy-turviness of the quiver means precisely that A_{eo} is the opposite of A_{oe}. We thus obtain a graph with vertices $V_{even} \cup V_{odd}$, and with edges between V_{even} and V_{odd}, such that directing edges from V_{even} to V_{odd} gives us A_{eo} and directing edges from V_{odd} to V_{even} gives us A_{oe}. This is a bipartite graph, by definition.
Reversing the above argument, from any bipartite quiver, we obtain a directed topsy-turvy quiver. □

Example 11 The bipartite graph $\bullet \!-\!\!-\!\!-\! \bullet$ with two vertices and a single edge results in a topsy-turvy quiver which can be depicted as an oriented line:

$$\cdots \qquad \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \qquad \cdots$$

The bipartite graph

results in a topsy-turvy quiver which can be depicted as a directed square lattice in $\mathbb{R}^2$:



The bipartite graph whose vertices are elements of the square lattice lattice in $\mathbb{R}^2$ results in a topsy-turvy quiver whose arrows can be thought of as the diagonals of a face-centred cubic lattice in $\mathbb{R}^3$.

5. SELF-INJECTIVE DIRECTED ALGEBRAS OF LENGTH ≤ 3

Throughout the following, let B be an indecomposable self-injective directed algebra. Here self-injective means that $B \cong \bigoplus_{x\in\Lambda} \mathrm{Hom}_F(Ae_x, F)$ as left B-modules or, equivalently, that all projective B-modules are also injective, and vice versa. Directed is understood to mean that the Ext^1-quiver of B is a directed quiver.
Note that such an algebra is necessarily infinite-dimensional, since directed implies quasi-hereditary which, in the finite-dimensional case, implies finite global dimension, contradicting self-injectivity.

LEMMA 12. *If B is radical-graded, all projective B-modules have the same Loewy length.*

Proof. For finite-dimensional algebras, this was shown in [12, Theorem 3.3]. We remark that the same proof holds for algebras in our setup, as the comparisons of Loewy length only need to be done using neighbouring projectives in the Ext-quiver. □

Let us now assume that B be an indecomposable self-injective algebra of Loewy length ≤ 3.

LEMMA 13. *B is radical-graded.*

Proof. Set $A_0 := \bigoplus\limits_{x\in\Lambda} Fe_x \cong A/\operatorname{Rad} A$ realized by the semisimple algebra generated by the idempotents, this is obviously a subalgebra. It acts naturally on the bimodule $A_1 \cong \operatorname{Rad} A/\operatorname{Rad}^2 A$ given by the arrows in the Ext-quiver and on $A_2 := \operatorname{Rad}^2 A$. Obviously the multiplication maps $A_1 \otimes A_1$ to A_2, so A is radical-graded. □

COROLLARY 14. *All projectives of B have the same Loewy length.*

LEMMA 15. *The quiver of B is a topsy-turvy quiver.*

Proof. A projective indecomposable B-module $P(\lambda)$ can be identified with an injective indecomposable B-module $I(\lambda^\phi)$. Here ϕ is a quiver isomorphism, corresponding to the Nakayama automorphism of B. Since B is selfinjective Loewy length 3, elements of $\mathcal{F}(\lambda)$ correspond to composition factors in the heart of $P(\lambda) =_B Be_\lambda$. Switching from left action to right action, we find elements of $\mathcal{P}(\lambda^\phi)$ correspond to composition factors in the heart of $e_\lambda B_B$. Taking duals, we find elements of $\mathcal{P}(\lambda^\phi)$ correspond to composition factors in the heart of $I(\lambda^\phi)$. Since $P(\lambda) = I(\lambda^\phi)$, we conclude $\mathcal{F}(\lambda) = \mathcal{P}(\lambda^\phi)$. Thus B has a topsy-turvy quiver, as required. □

To any topsy-turvy quiver Q, we can associate a self-injective algebra $R(Q)$ of Loewy length 3 by factoring out relations from the path algebra as follows: make products of arrows of Q which do not lie in some $\mathcal{F}(u) \cup \mathcal{P}(u^\phi)$ equal to zero; make squares in $\mathcal{F}(u) \cup \mathcal{P}(u^\phi)$ commute.
Let us now assume B is directed.

LEMMA 16. (a) *If B has Loewy length 2, it is isomorphic to the FQ/I, where Q is the infinite quiver*

$$\cdots \qquad \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \longrightarrow \bullet \qquad \cdots$$

and I is the quadratic ideal generated by all paths of length two.
(b) *If B has Loewy length 3, it is given by $R(Q)$, where Q is a directed, topsy-turvy quiver.*

Proof. (a) Obvious.
(b) Since projectives are injectives, both have irreducible head and socle. Since B is directed, projectives have structure

$$\begin{matrix} \lambda \\ \mu_1 \oplus \ldots \oplus \mu_n \\ \nu, \end{matrix}$$

where $\nu < \mu_i < \lambda$ all i. We only have to worry about the nonzero relations. These take the form $ac = \xi bd$, for $\xi \in F^\times$, where a, b are arrows in $F(u)$ and c, d are arrows in $P(u^\phi)$ for some u. We want to remove the scalars ξ from this description.
Let us write $B = FQ/I$. Then Q is topsy-turvy with ϕ described by the Nakayama automorphism of B. Since Q is directed as well, we can give the collection of vertices of our quiver a $\mathbb{Z}$-grading, so that arrows have degree 1, and ϕ has degree 2. We now alter scalars inductively. Arrows from vertices of degree 0 to vertices of degree 1 we leave alone. An arrow a from degree 1 to degree 2 lies in $P(t(a))$, and in no other $P(w)$. Therefore, multiplying arrows between vertices of degree 1 and degree 2 by nonzero scalars if necessary, we can force squares in quiver degree $0, 1, 2$ to commute. Similarly, multiplying arrows in degree $2, 3$ by scalars, we can force squares in quiver degree $1, 2, 3$

to commute. And so on. Working backwards, make squares in degree $-1, 0, 1$ commute and so on. □

Suppose Γ is a bipartite graph. The double quiver of Γ is the quiver which has vertices as Γ and a pair of opposing arrows running along each edge of Γ.

Definition 17. *Let B_Γ denote the self-injective directed algebra $R(Q_\Gamma)$. Let A_Γ denote the trivial extension $T(B_\Gamma)$ of B_Γ. Let $\mathcal{C}_\Gamma$ denote the category A_Γ-mod.*

We define Z_Γ to be the zigzag algebra associated to Γ [7]. It is the path algebra of the double quiver associated to Γ modulo relations insisting that all quadratic paths based at a single vertex are equal, whilst all other quadratic relations are zero. Since the relations are homogeneous, Z_Γ is a $\mathbb{Z}_+$-graded algebra with homogeneous elements graded by path length.

Lemma 18. *The category Z_Γ-mod is Calabi-Yau of dimension 0. We have an equivalence*

$$Z_\Gamma\text{-gr} \simeq B_\Gamma\text{-mod}^{\oplus 2}$$

between the category Z_Γ-gr of graded modules of Z_Γ, taken with respect to the $\mathbb{Z}_+$-grading by path length, and the direct sum of two copies of B_Γ-mod.
Under this equivalence, twisting by the automorphism ϕ of Q_Γ corresponds to a degree shift by 2 in Z_Γ-gr.

Proof. The irreducible objects of Z_Γ-gr are $S\langle i\rangle$, where S is an irreducible Z_Γ-module concentrated in degree 0. There are homomorphisms in Z_Γ-gr between $S\langle i\rangle$ and $T\langle j\rangle$ precisely when $S = T$ and $i = j$. There is an extension in Z_Γ-gr of $S\langle i\rangle$ by $T\langle j\rangle$ precisely when there is an extension between S by T in Z_Γ-mod and $j = i+1$. In particular when there exists such an extension, S corresponds to a vertex in V_l and T corresponds to a vertex in V_r. We thus have two blocks in Z_Γ-gr: one block is generated by $S\langle i\rangle$ where S lies in V_l and i is even or S lies in V_r and i is odd; the other block is generated by $S\langle i\rangle$ where S lies in V_r and i is even or S lies in V_l and i is odd. It is not difficult to see that each block is isomorphic to B_Γ-mod so that the automorphism ϕ corresponds to a degree shift $\langle 2\rangle$. □

For a quiver Q, we define P_Q to be the path algebra of Q, modulo the ideal of all paths of length ≥ 2.

Lemma 19. *For every orientation $\vec{\Gamma}$ of the bipartite graph Γ, we have an isomorphism*

$$Z_\Gamma \cong T(P_{\vec{\Gamma}})$$

between Z_Γ and the trivial extension algebra $T(P_{\vec{\Gamma}})$ of $P_{\vec{\Gamma}}$ by its dual.

Proof. Projectives for $P_{\vec{\Gamma}}$ take two shapes: they are either of Loewy length two, hence have a simple top with a certain number of extensions, or they are simple. Similarly injectives are simple in the first case or of length two with a simple socle and a certain number of simples in the top in the second case. Projectives for $T(P_{\vec{\Gamma}})$ are extensions of projectives for $P_{\vec{\Gamma}}$ by injectives for the same algebra, hence either of a module of Loewy length two with a certain number of simples in the socle by a simple or of a simple by a module of Loewy length two with a simple socle and some composition factors in the top. In both cases top and socle of the resulting extension have to be simple which forces, in the first case, all of the simples in the socle of the $P_{\vec{\Gamma}}$-projective to extend the simple $P_{\vec{\Gamma}}$-injective, and in the second case, the simple $P_{\vec{\Gamma}}$-projective to extend all the simples in the top of the $P_{\vec{\Gamma}}$-injective. This is the same as saying that for every arrow in $\vec{\Gamma}$ the quiver for $T(P_{\vec{\Gamma}})$ has an arrow in the opposite direction as well, and that all quadratic paths based at a single vertex are the same (we can easily get rid of scalars by rescaling the arrows) while all other quadratic relations are zero. This exactly describes the algebra Z_Γ. □

In this way, every orientation $\vec{\Gamma}$ of the graph Γ defines a $\mathbb{Z}_+^{\{f,a\}}$-grading on Z_Γ, whose f component corresponds to the $\mathbb{Z}_+$-grading of $P_{\vec{\Gamma}}$ by path length, and whose a component corresponds to the $\mathbb{Z}_+$-grading of $T(P_{\vec{\Gamma}})$ which puts $P_{\vec{\Gamma}}$ in degree 0 and its dual in degree 1.
Correspondingly, the orientation $\vec{\Gamma}$ of Γ gives rise to a $\mathbb{Z}_+^{\{f,a\}}$-grading of the associated selfinjective directed algebra B_Γ as follows: define a bigrading of the corresponding topsy-turvy quiver by grading arrows with an f if they run with the orientation $\vec{\Gamma}$ of Γ, and grading them a if they run against the orientation. This grading extends to a $\mathbb{Z}_+^{\{f,a\}}$-grading of B_Γ.

6. Hicas of length ≤ 4

The following is a classical statement which holds for any quasi-hereditary algebra:

Lemma 20. (a) ${}_A\Delta \cong (\nabla_A)^*$
(b) ${}_A\nabla \cong (\Delta_A)^*$

Lemma 21. *Suppose $\mathcal{C} = A$-mod is a highest weight category which is Calabi-Yau of dimension 0, and Ringel self-dual. Then A is quasi-hereditary with respect to two orders, denoted ▲ and ▼, and we have*

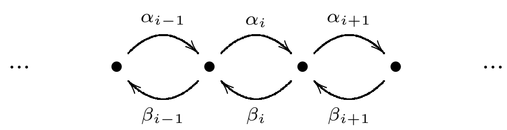
(a) ${}_A\Delta^{\blacktriangle} \cong {}_A\nabla^{\blacktriangledown}$
(b) ${}_A\Delta^{\blacktriangledown} \cong {}_A\nabla^{\blacktriangle}$

Proof. Let us suppose the quasi-hereditary structure on A is given by the partial order ▲, and the one induced by Ringel duality is ▼. Since A is Ringel self-dual, we have an isomorphism $A \cong A'$. Say that under this homomorphism the right projective e_xA corresponding to $x \in \Lambda$ goes to the right projective e'_yA' for some $y \in \Lambda$. Then by $\mathrm{Hom}_A(Ae_x, A) \cong e_xA \cong e'_yA' = \mathrm{Hom}_A(T(y), A)$ for $T(y)$ the tilting module for y and the fact that any projective for A is also injective and therefore tilting, it follows that $T(y) = P(x)$. So all tilting modules are projective A-modules. So, there is a 1-1-correspondence between tilting modules and projective modules for A, say it is, in the above scenario given by $y = \sharp x$. In particular this gives a one-to-one correspondence between standard modules and their socles $x = \operatorname{soc} \Delta^{\blacktriangle}(\sharp x)$. This makes the definition $\Delta^{\blacktriangledown}(x) := \nabla^{\blacktriangle}(\sharp x)$ well-defined. Filtrations of projectives by $\Delta^{\blacktriangledown}$s as well as the respective ordering conditions follow immediately from the dual statments for injectives (=projectives) and $\nabla^{\blacktriangle}$s. □

We wish to classify hicas of length ≤ 4. To warm up, let us classify hicas of length ≤ 3.

Lemma 22. *Hicas of length* 1 *are semisimple. There are no hicas of length* 2. *There is a unique hica of length* 3, *which is the module category of the Brauer tree algebra associated to a bi-infinite line.*

Proof. Length 1 hicas are trivially semisimple.
Suppose $\mathcal{C} = A$-mod is a hica of length 2. Standard objects in $\mathcal{C}$ must have length 2, since $\mathcal{C}$ is indecomposable, but not semisimple. Since $\mathcal{C}$ itself has length 2, all projective objects in $\mathcal{C}$ also have length 2. Thus standard objects are projective, and the socle of a projective indecomposable object Ae_x has irreducible summands indexed by elements y of Λ with $y < x$. Since A is a symmetric algebra, the top and socle of Ae_x are equal, which is a contradiction. Therefore there are no hicas of length 2.
Suppose $\mathcal{C} = A$-mod is a hica of length 3. Then $l({}_A\Delta) + l(\Delta_A) = 4$, by Lemma 6. We have $1 \leq l({}_A\Delta), l(\Delta_A) \leq 3$ since $\mathcal{C}$ has length 3. It is impossible that $l({}_A\Delta) = 3$, since this would imply standard objects are projective, leading to a contradiction as in the case when $\mathcal{C}$ is a hica of length 2. It is dually impossible that $l(\Delta_A) = 3$. Therefore $l({}_A\Delta) = l(\Delta_A) = 2$. The next step is to show our hica $\mathcal{C}$ of length 3 is Ringel self-dual. This follows just in the proof of Ringel duality for hicas of length 4 in Lemma 25 below: it is only necessary to replace the numbers 4 and 3 by the numbers 3 and 2. Since a standard object $\Delta(x)$ is a costandard object for some other ordering, by Lemma 21, $\Delta(x)$ must have an irreducible socle x_{-1}, as well as an irreducible top $x = x_0$. Likewise, x is the socle of some standard object $\Delta(x_1)$, for some $x_1 > x$. The projective Ae_x has a filtration whose sections are $\Delta(x_1)$ and $\Delta(x_0)$; it is not possible there are any other standard objects in a Δ-filtration since the existence of such would imply either the socle or top of Ae_x was not irreducible. We conclude Ae_x has top and socle isomorphic to x_i, and top modulo socle isomorphic to $x_{-1} \oplus x_1$. Inductively, we find $x_i \in \Lambda$, for $i \in \mathbb{Z}$, such that Ae_{x_i} has a filtration whose top and socle are isomorphic to x_i, and top modulo socle isomorphic to $x_{i-1} \oplus x_{i+1}$. It follows A is isomorphic to the path algebra of the quiver



modulo relations $\alpha_{i+1}\alpha_i = \beta_i\beta_{i+1} = 0$, and relations $\alpha_i\beta_i - \lambda_i\beta_{i+1}\alpha_{i+1} = 0$, for some nonzero $\lambda_i \in k$. Rescaling the generators if necessary, we may take all $\lambda_i = 0$. Thus A is isomorphic to the Brauer tree algebra associated to a bi-infinite line. $\square$

Let us now assume $\mathcal{C}$ is a hica of length 4. Thus $\mathcal{C} = A$-mod for a symmetric quasi-hereditary Δ-homogeneous algebra A of Loewy length 4.

Lemma 23. *The endomorphism ring of a projective indecomposable object in $\mathcal{C}$ is isomorphic to $F[d]/d^2$.*

Proof. The top and socle of a projective indecomposable are isomorphic, and such a simple cannot appear in either of the middle radical layers as this would imply a self-extension of the simple, contradicting quasi-heredity. $\square$

Lemma 24. *Either ${}_A\Delta$ has length 3 and Δ_A has length 2, or else ${}_A\Delta$ has length 2 and Δ_A has length 3.*

Proof. Since A is a hica, we have

$$l({}_A\Delta) + l(\Delta_A) = 5.$$

It is impossible that $l({}_A\Delta) = 1$ since this would imply that $A_A = \Delta_A$, which contradicts Lemma 23. Likewise it is impossible that $l(\Delta_A) = 1$. It follows that $\{l({}_A\Delta), l(\Delta_A)\} = \{2, 3\}$, as required. $\square$

We use $<$ to mean "less than, in the order $\blacktriangle$".

Lemma 25. *$\mathcal{C}$ is Ringel self-dual.*

Proof. To say that $\mathcal{C}$ is Ringel self-dual is to say that ${}_AA$ is a full tilting module for A. This is equivalent to saying that A_A is a full tilting module for A (consider finite dimensional quotients/subalgebras, and pass to a limit). In other words, A is left Ringel self-dual if and only if A is right Ringel self-dual. To establish the Ringel self-duality of $\mathcal{C}$, we may therefore assume that ${}_A\Delta$ has length 3, by Lemma 24.

Suppose $\mathcal{C}$ is not Ringel self-dual. Then we have a nonprojective indecomposable tilting module $T(\lambda)$, which has a filtration with sections

$$\Delta(\lambda), \Delta(\lambda_2), ..., \Delta(\lambda_n).$$

Note that $\Delta(\lambda)$ is the bottom section, and up to scalar we have a unique homomorphism from $P(\lambda)$ to T whose image is $\Delta(\lambda)$ (reference Ringel). Since T is nonprojective, it has length < 4. Since the sections all have length 3, the tilting module has length 3, and the tops of the sections all lie in the top of T. The module T also has a ∇-filtration since it is tilting. Any simple in the top of T must lie in the top of some ∇ of length 2. In particular, λ itself must lie in the top of some $\nabla(\mu)$ of length 2. The resulting homomorphism $P(\lambda) \to \nabla(\mu)$ must lift to a homomorphism $P(\lambda) \to T$. Up to scalar, there is a unique such homomorphism whose image is $\Delta(\lambda)$, implying that μ is a factor of $\Delta(\lambda)$. Thus, λ is a factor of $\nabla(\mu)$ and μ is a factor of $\Delta(\lambda)$. Thus $\lambda > \mu > \lambda$ which is a contradiction. $\square$

Lemma 26. *Standard modules for A have irreducible head and socle.*

Proof. A standard module in one ordering is isomorphic to a costandard module in another ordering, by Lemmas 21 and 25. □

If there is a nonsplit extension of λ by μ then either $\lambda > \mu$ or $\lambda < \mu$. We define *Rel* to be the set of relations $\lambda > \mu$ or $\lambda < \mu$ of this kind. We define $\uparrow$ to be the partial order on Λ generated by *Rel*. The order $\blacktriangle$ is a refinement of $\uparrow$.
We define $\downarrow$ to be the ordering on Λ which is Ringel dual to $\uparrow$.

Lemma 27. *$\mathcal{C}$ is a highest weight category with respect to the partial order $\uparrow$ on Λ.*

Proof. $\mathcal{C}$ has length 4, which implies that either left or right standard modules have length two and, by Lemma 26, are therefore uniserial. The quasi-hereditary structure induced by $\blacktriangle$ is already determined by these non-split extensions and therefore the order $\uparrow$ already induces the same quasi-hereditary structure as its refinement $\blacktriangle$. □

From now on, whenever we refer to standard or costandard modules, or to orderings, without specifying the order, we mean the order $\uparrow$.
We say an A-module M is *directed*, if given a subquotient of M which is a non-split extension of a simple module λ by a simple module μ, λ is greater than μ.

Lemma 28. *Standard A-modules are directed.*

Proof. We want that all standard modules are directed, which means for any subquotient of a standard module which is a non-split extension of simple modules λ by μ, λ is greater than μ. This is trivial for a standard module of Loewy length 2.
Let $\Delta(x)$ be a standard module of Loewy length 3. It must have an irreducible socle y by Lemma 26. Thus $\Delta(x)$ appears in a Δ-filtration of $P(y)$. $\Delta(y)$ appears as the top factor of a Δ-filtration of $P(y)$. Indeed, since $P(y)$ has length 4 with irreducible top and socle, a Δ-filtration of $P(y)$ has precisely two factors, namely $\Delta(x)$ and $\Delta(y)$.
The module $\Delta(y)$ must have irreducible socle z, where $y > z$, by Lemma 26. Since $P(y)$ has length 4 and $\Delta(y)$ has length 3, we conclude there is an extension of z by y. Since $\nabla(y)$ is dual to a Δ which has length 2, $\nabla(y)$ itself has length 2, and it must in fact be this extension of z by y.
For any other nonsplit extension of an irreducible modules w by y, we must have $w > y$ by Lemma 27. These are precisely the extensions of w by y contained in $\Delta(x)$. The extensions of x by w contained in $\Delta(x)$ imply $x > w$ by definition of a standard module. Thus any extension of λ by μ in $\Delta(x)$ implies $\lambda > \mu$ as required. □

Corollary 29. *The orders $\uparrow$ and $\downarrow$ on Λ are opposite.*

Proof. Just as standard modules are directed in the $\uparrow$ ordering, costandard modules are directed in the $\downarrow$ ordering. But standard modules in the $\uparrow$ ordering are equal to costandard modules in the $\downarrow$ ordering by Lemmas 21 and 25. Therefore $\uparrow$ and $\downarrow$ orderings are opposite, as required. □

Remark 30 If a finite-dimensional algebra is quasi-hereditary with respect to two opposing orders then it must be directed, in which case the standard modules are projectives in one ordering, and simples in the opposite ordering. This can easily be proved by induction on the size of the indexing set. Symmetric quasi-hereditary algebras are never directed, since their projective indecomposable objects have isomorphic head and socle.

Remark 31 It is not necessarily the case that a Ringel self-dual hica is a highest weight category with respect to two opposing orderings. Examples of length 5 are found amongst module categories of rhombal algebras [3].

Let $X(\lambda)$ denote the kernel of the surjective homomorphism $\Delta(\lambda) \twoheadrightarrow \lambda$, for $\lambda \in \Lambda$.

Definition 32. *The* Δ-quiver *of A is the quiver with vertices indexed by Λ, and with arrows $\lambda \to \mu$ corresponding to simple composition factors μ in the top of $X(\lambda)$.*

Lemma 33. *Components of the Δ-quiver of length 2 are directed lines. Components of the Δ-quiver of length 3 are directed topsy-turvy quivers.*

Proof. The length 2 case is easy.
In length 3, we have a permutation $\phi \circlearrowleft \Lambda$ which takes λ to the socle of $\Delta(\lambda)$. We prove that $\mathcal{F}(\lambda) = \mathcal{P}(\lambda^{\phi})$ via a sequence of correspondences: arrows emanating from λ in the Δ-quiver are in correspondence with simple composition factors μ in the top of $X(\lambda)$; simple composition factors μ in the top of $X(\lambda)$ are in correspondence with extensions of λ by μ such that $\lambda > \mu$; since $\Delta^{\uparrow}(\lambda) = \nabla^{\downarrow}(\lambda^{\phi})$, whilst $\uparrow$ and $\downarrow$ are opposites, extensions of λ by μ such that $\lambda > \mu$ are in one-one correspondence with extensions of μ by λ^{ϕ} such that $\mu > \lambda^{\phi}$; extensions of μ by λ^{ϕ} such that $\mu > \lambda^{\phi}$ are in correspondence with simple composition factors λ^{ϕ} in the top of $X(\mu)$; simple composition factors λ^{ϕ} in the top of $X(\mu)$ are in one-one correspondence with arrows into λ^{ϕ} in the Δ-quiver.
Since standard modules are directed, the Δ-quivers are also directed (ie they generate a poset). □

We next find Δ-subalgebra of A, in the sense of S. Koenig [10].

Lemma 34. *A has a Δ-subalgebra B.*

Proof. We want to find B such that ${}_B\Delta \cong {}_BB$. Let us write $A = FQ/I$ as the path algebra of Q modulo relations, where Q is the Ext^1-quiver of A. If there is a *positive* arrow $x \to y$ in Q, that is to say an arrow $x \to y$ in Q such that $x > y$, then x and y lie in the same component of the Δ-quiver. Since all standard modules are directed, the connected component of the quiver generated by these arrows are the components of the Δ-quiver.
Let B be the subalgebra of A generated by arrows $x \to y$ in Q such that $x > y$. Since all standard modules are directed, composing the natural maps

$Be_\lambda \to Ae_\lambda \to \Delta(\lambda)$ gives us a surjection $Be_\lambda \twoheadrightarrow \Delta(\lambda)$. To establish this composition map is an isomorphism, we have to worry about its kernel, which must lie in $\mathrm{Rad}^2(B)e_\lambda$, which is the socle of B since A has length 4. Assume there is a simple S in the kernel. Then S would have to be a factor of $\Delta(\mu)$ in a Δ-filtration of Ae_λ; restrictions imply S would lie in the socle of some $\Delta(\mu)$ of length 2, where $\mu > \lambda$ (otherwise if $\Delta(\mu)$ has length 3 then λ lies in the socle of $\Delta(\mu)$ so $S > \lambda$, $\lambda > S$ since S appears in Be_λ, contradiction). Since S lies in $\mathrm{Rad}^2(B)e_\lambda$, we have positive arrows $\lambda \to \nu \to S$, for some ν, so S must lie in $\Delta(\nu)$, and there is an arrow $\lambda \to \nu$ in the Δ-component of λ. There are now two possibilities. Either $\Delta(\lambda)$ has length 3, implying S lies in a Δ-quiver component of length 2 (for μ), and a Δ-quiver component of length 3 (for λ)- contradiction. Else $\Delta(\lambda)$ has length 2, which implies we have a Δ-quiver component of length 2 containing the quiver $\mu \to S \leftarrow \nu$ - contradiction (the structure of any length 2 Δ-quiver component is an oriented line by Lemma 33). We conclude that the map $B \twoheadrightarrow \Delta$ must in fact have zero kernel, ie B is a Δ-subalgebra.

□

Let B be the Δ-subalgebra of A.

Lemma 35. *Suppose B has length 3. Then the algebra homomorphism $B \to A$ splits.*

Proof. Let I denote the ideal of A which is a sum of spaces AaA where a is a *negative* arrow in the quiver Q of A. Then the kernel J of the A-module homomorphism $A \to {}_A\Delta$ is contained in I, since A has length 4 and Δs have length 3, implying J is generated in the top of the radical of A. Also, J contains I since I is generated as a vector space by products of 1, 2, or 3 arrows in the quiver, at least one of which lies in I, and these products all lie in J since all Δs are directed. Thus the kernel of $A \to {}_A\Delta$ is equal to I. By symmetry, the homomorphism of right A-modules $A \to \Delta_A$ also has kernel I. Therefore $B \oplus I \to A$ is an isomorphism of B-B-bimodules, and the algebra homomorphisms

$$B \to A \to A/I$$

compose to give an algebra isomorphism $B \cong A/I$. Therefore the homomorphism $B \to A$ splits as required. □

Lemma 36. *B is self-injective.*

Proof. We write ${}^\uparrow B$ for the ${}_A\Delta$-subalgebra taken with respect to the $\uparrow$ ordering, and $B^\downarrow$ the Δ_A-subalgebra taken with respect to the $\downarrow$ ordering. We know that

$$B = {}^\uparrow B \cong \bigoplus_{x\in\Lambda} {}_A\Delta^\uparrow(x) \cong \bigoplus_{x\in\Lambda} {}_A\nabla^\downarrow(x) \cong \bigoplus_{x\in\Lambda} (\Delta^\downarrow_A(x))^* \cong (B^\downarrow)^*,$$

where $B^\downarrow$ is also a Δ-subalgebra of A. Thus ${}^\uparrow B \cong (B^\downarrow)^*$ as A-modules, and therefore as ${}^\uparrow B$-modules. To prove ${}^\uparrow B$ is self-injective we must show that ${}^\uparrow B \cong B^\downarrow$. Indeed, ${}^\uparrow B$ is defined to be the subalgebra generated by left positive

$\uparrow$-arrows, whilst $B^{\downarrow}$ is defined to be the subalgebra generated by right positive $\downarrow$-arrows. Passing from the left regular action of an algebra on itself to the right regular action reverses arrow orientation. Therefore left positive $\uparrow$-arrows are equal to right negative $\uparrow$-arrows which are equal to right positive $\downarrow$-arrows. Thus ${}^{\uparrow}B \cong B^{\downarrow}$ as required. $\square$

Lemma 37. *If B has Loewy length 3, then A is isomorphic to $T(B)$, the trivial extension algebra of B by its dual.*
If B has Loewy length 2, then A is isomorphic to $U(B, M)$ where M is a self-dual B-B-bimodule.

Proof. We may assume $B = B^{\uparrow}$ has Loewy length 3, in which case $B^{\downarrow}$ has Loewy length 2. We have a surjection of algebras $A \twoheadrightarrow B$ which splits, via an algebra embedding $B \hookrightarrow A$. Dually, we have an embedding of A-A-bimodules $B^* \hookrightarrow A^*$. Since $A \cong A^*$ as bimodules, we have a homomorphism of A-A-bimodules $B^* \hookrightarrow A$. Taking the sum of our two embeddings gives us a homomorphism of B-B-bimodules,

$$B \oplus B^* \to A.$$

This homomorphism is a bimodule isomorphism, because every projective indecomposable A-module has a canonical Δ-filtration featuring precisely two $\Delta(\lambda)$s, one of which is a summand of B, and the other of which is a summand of B^*. We can thus identify the image of B^* in A with the kernel of the algebra homomorphism $A \to B$. The image of B^* in A multiplies to zero, because the map $B^* \to A$ is a homomorphism of A-A-bimodules, on which the kernel of the surjection $A \twoheadrightarrow B$ acts trivially. The image of B in A multiplies via according to multiplication in B. In other words, the map $T(B) = B \oplus B^* \to A$ is an algebra isomorphism, as required.
The algebra A has a $\mathbb{Z}_+^2$-grading whose first component comes from the radical grading on $B^{\uparrow}$, and whose second component comes from the trivial extension grading, with $B^{\uparrow}$ in degree 0 and its dual in degree 1. In other words, the degree $(*, 0)$ part of A is $B^{\uparrow}$. We can then identify the degree $(0, *)$ part of A with $B^{\downarrow}$, which is self-injective of Loewy length 2. The degree $(2, *)$ part of A is then isomorphic to $B^{\downarrow *}$, and we define M to be the degree $(1, *)$ part of A. The isomorphism $A \cong A^*$ exchanges the $B^{\downarrow}$-$B^{\downarrow}$-bimodules $B^{\downarrow}$ and $B^{\downarrow *}$, whilst it defines an isomorphism $M \cong M^*$. This way, we obtain the algebra isomorphism $A \cong U(B^{\downarrow}, M)$. $\square$

Let $\mathfrak{Bip}$ denote the 2-category whose objects are bipartite graphs; whose arrows $\Gamma \to \Gamma'$ are given by sequences $(\gamma_1, ..., \gamma_n)$ of distinct vertices of Γ, such that $\Gamma' = \Gamma \backslash \{\gamma_1, ..., \gamma_n\}$; whose 2-arrows are given by permutations of such sequences.
The following result is a refinement of Theorem 1.

Theorem 38. *The correspondence $\Gamma \mapsto \mathcal{C}_{\Gamma}$ extends to a 2-functor*

$$\mathfrak{Bip} \to \mathfrak{Hica}_4$$

which is essentially bijective on objects.

Proof. The correspondence $\Gamma \mapsto A_\Gamma$ -mod is essentially bijective on objects, by Lemmas 16, 34, 36, and 37.
We have to associate functors and natural transformations in $\mathfrak{Hica}_4$ to arrows and 2-arrows in $\mathfrak{Bip}$. Suppose $\gamma \in \Gamma$ is a vertex of a bipartite graph, and $\Gamma' = \Gamma \backslash \gamma$. We have an isomorphism $A_{\Gamma'} \cong e_{\Gamma'} A_\Gamma e_{\Gamma'}$, and therefore an exact functor

$$F_\gamma = e_{\Gamma'} A_\Gamma \otimes_{A_\Gamma} : A_\Gamma\text{-mod} \to A_{\Gamma'}\text{-mod}$$

which sends the irreducible corresponding to a vertex v to the irreducible corresponding to a vertex v, if $v \neq \gamma$ and to zero if $v = \gamma$. To a sequence $(\gamma_1, ..., \gamma_n)$ we associate the composition functor $F_{\gamma_n} ... F_{\gamma_1}$. There are natural isomorphisms between various functors corresponding to isomorphisms of bimodules. □

Let $B^\uparrow = FQ^\uparrow / R^\uparrow$, $B^\downarrow = FQ^\downarrow / R^\downarrow$ be minimal presentations of $B^\uparrow$ and $B^\downarrow$ by quiver and relations.
Let Q be the union of $Q^\uparrow$ and $Q^\downarrow$ in which we identify the vertices of these quivers if they represent the same irreducible A-module. Let R be the union of $R^\uparrow$, $R^\downarrow$ and $R^\updownarrow$. Let $R^\updownarrow$ denote the set of relations which insist that squares in Q involving two arrows of $Q^\uparrow$ and two arrows of $Q^\downarrow$ commute.

Lemma 39. *$A = FQ/R$ is a minimal presentation of A by quiver and relations.*

Proof. We have a surjective map $FQ \twoheadrightarrow A$. It is not difficult to see this must factor through a map $FQ/R \twoheadrightarrow A$. We now want to bound the dimension of a projective of FQ/R. Without loss of generality assum that $B = B^\uparrow$ has Loewy length 3 and $B^\downarrow$ therefore has Loewy length 2. So $Q^\uparrow$ is a topsy-turvy quiver and $Q^\downarrow$ is linear. We claim that a spanning set of $(FQ/R)e_x$ is given by abe_x where $b \in B$ and a is either an idempotent or an arrow from $Q^\downarrow$. Without a doubt a spanning set is given by the union of all elements of the form $a_1 b_1 \cdots a_r b_r e_x$ where a_i are either idempotents or arrows in $Q^\downarrow$ and $b_i \in B$. However, if we have an arrow a in $Q^\downarrow$ (say with source y and target $\phi^{-1}(y)$) and and arrow $b \in Q^\uparrow$ starting in $\phi^{-1}(y)$, the product $bae_y = be_{\phi^{-1}y} ae_y$ equals $a'b'e_y$ where $b' = \phi(b)$ and a' is the unique arrow starting at the end vertex of $b'e_y$. Indeed, $Q^\uparrow$ being topsy turvy implies the existence of b' and in $Q^\downarrow$ there is an arrow from x to $\phi^{-1}x$ for every x. So denoting by z the end vertex of b, there is a square

$$\begin{array}{ccc} y & \xrightarrow{a} & \phi^{-1}(y) \\ \downarrow{\scriptstyle \phi(b)} & & \downarrow{\scriptstyle b} \\ z & \xrightarrow{a'} & \phi^{-1}(z) \end{array} .$$

By the required relations this has to commute and we obtain $bae_y = a'b'e_y$. Hence the path $a_1 b_1 \cdots a_r b_r e_x$ is equivalent modulo R to a path $a'_1 \cdots a'_r b'_1 \cdots b'_r = a'_1 \cdots a'_r b'$. However, by the relations in $B^\downarrow$, any product of arrows in $Q^\downarrow$ is zero, so we obtain the claim that $(FQ/R)e_x$ is spanned by abe_x where $b \in B$ and a is either an idempotent or an arrow from $Q^\downarrow$.

This implies that $\dim(FQ/R)e_x \leq 2\dim Be_x = \dim(B+B^*)e_x = \dim Ae_x$, the equality $\dim Be_x = \dim(B+B^*)e_x$ coming from the fact that B is self-injective. Combining the above surjection $FQ/R \twoheadrightarrow A$ and this inequality, we obtain the statment of the lemma. □

7. Koszulity

For an algebra C we denote by $C^!$ the quadratic dual of C.

Theorem 40. *The following are equivalent:*

1. Γ *is not a simply laced Dynkin graph.*
2. Z_Γ *is Koszul.*
3. B_Γ *is Koszul.*
4. A_Γ *is Koszul.*
5. $A^!_\Gamma$-mod *is Calabi-Yau of dimension* 3.

The length of the proof of this result is the length of the section.

1 is equivalent to 2, by a theorem of Martínez-Villa [11].

2 is equivalent to 3, since B_Γ-mod$^{\oplus 2}$ is equivalent to Z_Γ-gr by Lemma 18.
The implication $3 \Rightarrow 4$ follows from the following lemma, in case $A = A_\Gamma$, and $B = B_\Gamma$.

Lemma 41. *If B is a self-injective Koszul algebra of length n, the trivial extension algebra $A = B \oplus B^*\langle n\rangle$ is Koszul.*

Proof. Since B is selfinjective, we have an isomorphism $B \cong B^*$ of B-modules. The algebra A is a trivial extension $A = B \oplus B^*$, and we thus have a map $A \to A$ of B-modules extending to a map of A-modules whose kernel is B^* and whose cokernel is B. Stringing these together gives us a projective resolution

$$... \to A \to A \to B$$

of B as a left A-module. Since B is self-injective and radical graded, every injective B-module has length n, and consequently this is a linear resolution of B as a left A-module. Taking summands, we find that every projective B-module has a linear resolution as a left A-module.
If B is Koszul, then B^0 has a linear resolution by projective B-modules. Thus B^0 is quasi-isomorphic to a linear complex of projective B-modules. Since projective B-modules are quasi-isomorphic to a linear complex of projective A-modules, we deduce B^0 is isomorphic to a linear complex of projective A-modules. That is to say, $A^0 = B^0$ has a linear resolution by projective A-modules. In other words, A is Koszul. □

The implication $4 \Rightarrow 3$ follows from the following lemma, in case $A = A_\Gamma$, and $B = B_\Gamma$.

Lemma 42. *If B is a radical-graded selfinjective algebra of length n, such that $A = B \oplus B^*\langle n\rangle$ is Koszul, then B is Koszul.*

Proof. We have a $\mathbb{Z}_+ \times \mathbb{Z}_+$-grading on A in which B lies in degree $(?, 0)$, the dual of B lies in degree $(?, 1)$, and in which the inherent $\mathbb{Z}_+$-grading on B is the radical grading. This corresponds to the action of a two-dimensional torus $\mathbb{T}$ on A. Thus $\mathbb{T}$ acts on A^1 and we have an exact sequence

$$0 \to R \to A^1 \otimes_{A^0} A^1 \to A^2 \to 0$$

of $\mathbb{T}$-modules, where R denotes the relations for A and A^j refers to the jth component in the total grading, whose dual

$$0 \leftarrow A^{!2} \leftarrow A^{!1} \otimes_{A^{!0}} A^{!1} \leftarrow R^! \leftarrow 0$$

is also an exact sequence of $\mathbb{T}$-modules. Since $A^!$ is quadratic by definition, with relations $R^!$, we have an action of $\mathbb{T}$ on $A^!$, which gives a $\mathbb{Z}_+ \times \mathbb{Z}_+$-grading on $A^!$. We have a linear resolution of $W = A^{(0,0)}$, given by the Koszul complex

$$A \otimes_W A^{!*}$$

of A ([1], 2.8). Here $A^{!*}$ denotes the graded dual of $A^!$. The differential on the Koszul complex respects the $\mathbb{Z}_+ \times \mathbb{Z}_+$-grading on A and $A^!$ (see [1], 2.6). In other words, it sends terms involving arrows in $A^{(0,1)}$ or $A^{!(0,1)*}$ to terms involving arrows in $A^{(0,1)}$ or $A^{!(0,1)*}$, and terms not involving arrows in $A^{(0,1)}$ or $A^{!(0,1)*}$ to terms not involving arrows in $A^{(0,1)}$ or $A^{!(0,1)*}$. Consequently the subcomplex $A^{(?,0)} \otimes_R A^{!(-,0)*})$ is a direct summand of the Koszul complex regarded as a complex of B-modules. Taking this component gives us a linear resolution of $R = B^0$ as a B-module. Therefore B is Koszul. $\square$

If C is a graded algebra and C-mod is Calabi-Yau of dimension n, then $Ext^*_C(C^0, C^0)$ is a super-symmetric algebra concentrated in degrees $0, 1, ..., n$, by Van den Bergh A.5.2 [2]. We have a converse which applies for Koszul algebras:

Theorem 43. *Suppose K is a Koszul algebra such that $K^!$ is super-symmetric of length $n+1$, then K-mod is Calabi-Yau of dimension n.*

Proof. There is an equivalence between derived categories of graded modules for $K^!$ and K via the Koszul complex. Since $K^!$ is locally finite dimensional, this restricts an equivalence of bounded derived categories, by a theorem of Beilinson, Ginzburg, and Soergel ([1], Theorem 2.12.6). Under this equivalence, simple $K^!$-modules correspond to projective indecomposable K-modules. Since $K^!$ is locally finite-dimensional The equivalence therefore restricts to an equivalence between $D^b(K^!\text{-gr})$ and $D^b(K\text{-grperf})$. Also under this equivalence, injective $K^!$-modules correspond to simple K-modules, whilst shifts $\langle i \rangle$ in $D^b(K^!\text{-gr})$ correspond to shifts in degree $\langle -i \rangle[-i]$ in $D^b(K\text{-grperf})$. This homological shift in degree means that the Calabi-Yau-n property for K-mod is equivalent to the super-Calabi-Yau-0 property for $K^!$-perf, thanks to Van den Bergh's calculation A.5.2 [2]. To prove the super-Calabi-Yau-0 property for $K^!$-perf, it is enough to check that $K^!$ is a super-symmetric algebra (cf [17], Theorem 3.1). $\square$

Assume 4. Then the Koszul dual $A^!$ of A is Calabi-Yau of dimension 3. The Koszul dual of a supersymmetric algebra of length $n+1$ is Calabi-Yau of dimenion n by Theorem 43. The trivial extension algebra $A = B + B^*\langle 3\rangle$ is super-symmetric with B concentrated in degrees $0, 1, 2$, with $B^*\langle 3\rangle$ concentrated in degrees $3, 2, 1$, and with bilinear form pairing B^i and $(B^i)^*\langle 3\rangle$ via

$$< \beta, b >= \beta(b) \qquad < b, \beta >= (-1)^{i(3-i)}\beta(b),$$

for $b \in B^i$, $\beta \in (B^i)^*$. Thus 4 implies 5.

Assume 5. Since $A^!$ is Calabi-Yau of dimension 3, its relations are the derivatives of a superpotential, and its degree 0 part has a 4-term resolution, its Jacobi resolution [2]. The superpotential must be cubic, since $A^!$ is quadratic. This implies further that the Jacobi resolution of $A^{!0}$ is linear, so $A^!$ must be Koszul. Thus 5 implies 4.

We have now shown that $1 \Leftrightarrow 2 \Leftrightarrow 3 \Leftrightarrow 4 \Leftrightarrow 5$, completing the proof of Theorem 40.

Remark 44 If Γ is a bipartite graph, then an orientation of Γ gives rise to a $\mathbb{Z}^3_+$-grading on A_Γ. If every vertex of Γ is attached to at least two vertices, then this leads to a $\mathbb{Z}^3_+$-grading of the Calabi-Yau algebra $A^!$ of dimension 3, which can otherwise be thought of as the action of a 3-dimensional torus on $A^!$. The algebra $A^!$ has homological dimension 3, and admits the action of a 3-dimensional torus. It thus belongs to the realm of 3-dimensional noncommutative toric geometry.

Example 45 If Γ is given by tiling of a bi-infinite line

$$\cdots \qquad \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \qquad \cdots$$

then the Calabi-Yau algebra of dimension 3 we obtain is familiar from toric geometry. It is the algebra associated to the brane tiling of the plane by hexagons [6]. Its quiver can be thought of as an orientation of the A_2-lattice (for a picture, see section 8, assumption 3). If we give Γ an alternating orientation,

$$\cdots \qquad \bullet \longleftarrow \bullet \longrightarrow \bullet \longleftarrow \bullet \longrightarrow \bullet \longleftarrow \bullet \longrightarrow \bullet \qquad \cdots$$

then in the resulting grading on $A^!$, the three copies of $\mathbb{Z}_+$ correspond to the three directions of arrows in the A_2-lattice.

8. Relaxing the assumptions

We have given a combinatorial classification of hicas of length ≤ 4 by bipartite graphs. Here we show that the relaxation of any of the homological assumptions on our categories would necessarily introduce further combinatorial complexity into the classification.

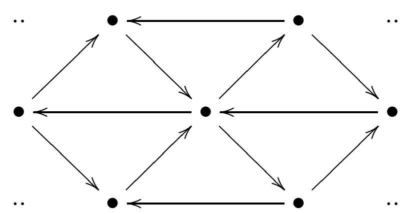
Assumption 1: highest weight structure.

The existence of a highest weight structure on a category is a strong assumption, and the assumptions of Ringel self-duality and homogeneity of standard modules require the existence of a highest weight structure on the category. It is a cinch to give examples of indecomposable Calabi-Yau 0 categories of length 4 which are not highest weight categories, such as the module category of the local symmetric algebra $F[x]/x^4$.

Assumption 2: Calabi-Yau 0 *property.*
The Calabi-Yau property is another strong homological restriction on a category. An example of a length 4 highest weight category which is indecomposable and Ringel self-dual, and whose standard modules are homogeneous, is the path algebra of the linear quiver

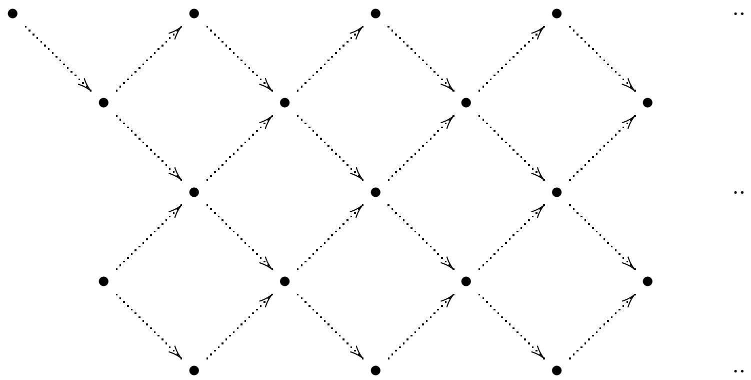
modulo all relations of degree ≥ 4.

Assumption 3: homogeneity.
The homogeneity restriction on a hica is fairly natural, since the known examples of highest weight Calabi-Yau 0 categories arising in group representation theory and the theory of tilings satisfy this restriction. However, some interesting combinatorics arise in length 4 if the condition is dropped.
For example, let $\mathcal{C}_\Gamma$ be the hica associated to a bi-infinite line Γ, whose quiver is an orientation

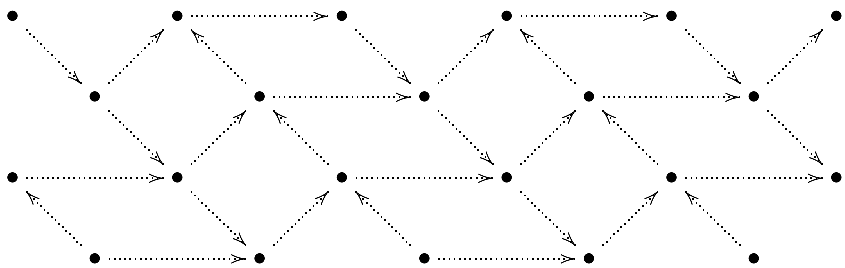


of the A_2 lattice, by example 45, and by construction comes with a (horizontal) projection π onto Γ.
There are two natural ways to obtain highest weight indecomposable Calabi-Yau 0 categories which are not homogeneous from $\mathcal{C}_\Gamma$. The first is by choosing a section of π, that is a path in the A_2 lattice which projects homeomorphically onto Γ via π. The elements of Λ to the right of the path form a coideal in the poset. Truncating $\mathcal{C}_\Gamma$ at this coideal gives us a highest weight category of length 4 which is CY-0, but not homogeneous (cf. [4], 3.5(b)). Such a truncation is not Ringel self-dual. Beneath is a portion of such a truncated poset, whose left edge defines an orientation of Γ. We use dotted arrows to represent directions in a partial order on the vertices of the lattice, rather than solid arrows which

represent arrows in a quiver:



The second way to obtain an inhomogeneous highest weight indecomposable Calabi-Yau 0 category from $\mathcal{C}_\Gamma$ is by merely altering the ordering of the vertices. Certain orderings of the vertices of the A_2 lattice give A_Γ-mod is an inhomogeneous highest weight category, which is Ringel self-dual. Here is an example of a portion of such a partial ordering:



Assumption 4: length ≤ 4.
We have studied hicas of length 4, since 4 is the shortest length in which a nontrivial classification is possible. There are two kinds of hicas of length 5: those whose left and right standard modules have length 4 and 2, and those whose left and right standard modules have length 3 and 3.
The category of graded modules over a radical-graded symmetric algebra of length 4 is equivalent to the category of modules over a directed self-injective algebras of length 4. Trivial extensions of directed self-injective algebras of length 4 by their duals give examples of hicas of length 5 whose left and right standard modules have length 4 and 2.
Michael Peach's rhombal algebras give examples of hicas of length 5 associated to rhombic tilings of the plane whose left and right standard modules have length 3 and 3.
We would be interested to learn more about hicas of length 5.

9. Tilting

There are natural self-equivalences of the derived categories of $\mathcal{C}_\Gamma$, which are obtained from a standard tilting procedure for symmetric algebras:

Lemma 46. *Suppose A is a symmetric algebra, and suppose that the endomorphism ring $e_\lambda A e_\lambda$ is isomorphic to the dual numbers $F[d]/d^2$. Then we have an exact self-equivalence ψ_λ of the derived category of A given by tensoring with the two-term complex*

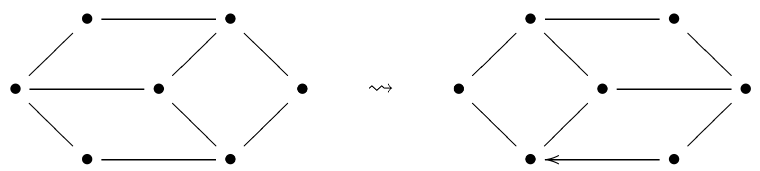
$$Ae_\lambda \otimes_F e_\lambda A \to A,$$

whose arrow is the multiplication map.

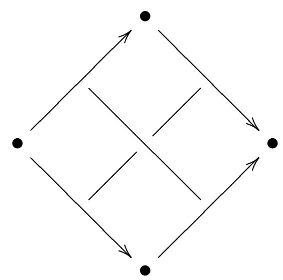
Proof. This functor is obviously exact. It fixes all simple modules with the exception of the simple top λ of Ae_λ, which it sends to $\Omega(\lambda)$. The module $\Omega(\lambda)$ has simple socle λ since A is symmetric, and other composition factors different from λ since $e_\lambda A e_\lambda$ is isomorphic to the dual numbers. Therefore collection of simples $\mu \neq \lambda$, along with Ω generate $D^b(A\text{-mod})$, and ψ_λ is an equivalence. □

The self-equivalence ψ_λ is called a spherical twist, because the cohomology ring of the sphere can be identified with the dual numbers (cf. [19]).
One way to obtain self-equivalences of $D^b(\mathcal{C}_\Gamma)$ from spherical twists is by lifting self-equivalences of the derived category of the zigzag algebra Z_Γ, whose projective indecomposable modules for the algebra Z_Γ all have an endomorphism ring isomorphic to the algebra of dual numbers. A second way to obtain self-equivalences of $D^b(\mathcal{C}_\Gamma)$ is to apply spherical twists directly to $\mathcal{C}_\Gamma$, whose projective indecomposable objects also have endomorphism rings isomorphic to the dual numbers.
Let us consider the first case. The projective indecomposable modules for the algebra Z_Γ all have an endomorphism ring isomorphic to the algebra of dual numbers. Standard tilts generate an action of a 2-category $\mathcal{T}_\Gamma$ on $D^b(Z_\Gamma\text{-gr})$ which lifts to an action of $\mathcal{T}_\Gamma$ on $D^b(\mathcal{C}_\Gamma)$, by a result of Rickard [16, Thm 3.1]. A second way to obtain self-equivalences of $D^b(\mathcal{C}_\Gamma)$ is to apply Seidel-Thomas twists directly to A_Γ, whose projective indecomposable modules have endomorphism rings isomorphic to the dual numbers. Standard tilts generate the action of a 2-category $\mathcal{U}_\Gamma$ on $D^b(\mathcal{C}_\Gamma)$, whose combinatorics is rather different from that of $\mathcal{T}_\Gamma$.

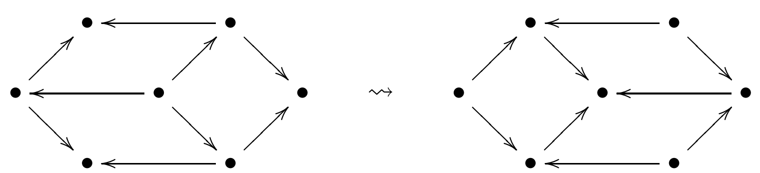
Example 47 When Γ is a bi-infinite line, we have an action of the braid 2-category $\mathcal{BC}_\infty$ on a bi-infinite line on the derived category of Z_Γ, by a theorem of Seidel and Thomas [9]. The action of $\mathcal{BC}_\infty$ on $D^b(Z_\Gamma\text{-mod})$ lifts to an action of $\mathcal{BC}_\infty$ on $\mathcal{C}_\Gamma$. Arrows in $\mathcal{BC}_\infty$ are braids with an infinite number of strands, and 2-arrows are braid cobordisms, such as Reidemeister moves pictured as follows:



In this picture, a rhombus represents a pair of braids running parallel to the two sides and crossing in the middle.



We have a natural 2-functor $\mathcal{BC}_\infty \to \mathcal{T}_\Gamma$. The Reidemeister move depicted above therefore corresponds in a natural way to a 2-*arrow* in $\mathcal{T}_\Gamma$. However, this Reidemeister move also corresponds naturally to an *arrow* in $\mathcal{S}_\Gamma$. Let us explain how. Suppose we remove edges of the A_2-lattice to give a rhombic tiling T of the plane, whose edges lie in the quiver Q of A_Γ. We have a grading of A_Γ which places arrows in Q which are edges of T in degree 0 and arrows in Q which are not edges of T in degree 1. Let us denote by D_T the degree 0 part of A taken with respect to this tiling. The algebra A_Γ is a trivial extension of D_T by D_T^*. If T' is obtained from T by a Reidemeister move centred on the vertex λ,



then $D_{T'}$ is derived equivalent to D_T, because the complex of D_T-modules given by the sum of $D_Te_\lambda \otimes e_\lambda D_T \to D_T$ and $D_Te_\lambda \to 0$ is a tilting complex whose derived endomorphism ring is isomorphic to $D_{T'}$. This derived equivalence between D_T and $D_{T'}$ lifts to an equivalence of trivial extensions, that is to say a self-equivalence of $D^b(A_\Gamma\text{-mod}) = D^b(\mathcal{C}_\Gamma)$; this self-equivalence of $D^b(\mathcal{C}_\Gamma)$ is precisely the spherical twist ψ_λ.

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On Higher Order Estimates in Quantum Electrodynamics

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Abstract. We propose a new method to derive certain higher order estimates in quantum electrodynamics. Our method is particularly convenient in the application to the non-local semi-relativistic models of quantum electrodynamics as it avoids the use of iterated commutator expansions. We re-derive higher order estimates obtained earlier by Fröhlich, Griesemer, and Schlein and prove new estimates for a non-local molecular no-pair operator.

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1. Introduction

The main objective of this paper is to present a new method to derive higher order estimates in quantum electrodynamics (QED) of the form

$$\| H_{\mathrm{f}}^{n/2} (H + C)^{-n/2} \| \leqslant \text{const} < \infty \,, \tag{1.1}$$

$$\| [H_{\mathrm{f}}^{n/2} , H] (H + C)^{-n/2} \| \leqslant \text{const} < \infty \,, \tag{1.2}$$

for all $n \in \mathbb{N}$, where $C > 0$ is sufficiently large. In these bounds H_{f} denotes the radiation field energy of the quantized photon field and H is the full Hamiltonian generating the time evolution of an interacting electron-photon system. For instance, estimates of this type serve as one of the main technical ingredients in the mathematical analysis of Rayleigh scattering. In this context, (1.1) has been proven by Fröhlich et al. in the case where H is the non- or semi-relativistic Pauli-Fierz Hamiltonian [4]; a slightly weaker version of (1.2) has been obtained in [4] for all even values of n. Higher order estimates of the form (1.1) also turn out to be useful in the study of the existence of ground states in a no-pair model of QED [8]. In fact, they imply that every eigenvector of the Hamiltonian H or spectral subspaces of H corresponding to some bounded interval are contained in the domains of higher powers of H_{f}. This information

is very helpful in order to overcome numerous technical difficulties which are caused by the non-locality of the no-pair operator. In these applications it is actually necessary to have some control on the norms in (1.1) and (1.2) when the operator H gets modified. To this end we shall give rough bounds on the right hand sides of (1.1) and (1.2) in terms of the ground state energy and integrals involving the form factor and the dispersion relation.
Various types of higher order estimates have actually been employed in the mathematical analysis of quantum field theories since a very long time. Here we only mention the classical works [5, 11] on $P(\phi)_2$ models and the more recent articles [2] again on a $P(\phi)_2$ model and [1] on the Nelson model.
In what follows we briefly describe the organization and the content of the present article. In Section 2 we develop the main idea behind our techniques in a general setting. By the criterion established there the proof of the higher order estimates is essentially boiled down to the verification of certain form bounds on the commutator between H and a regularized version of $H_{\mathrm{f}}^{n/2}$. After that, in Section 3, we introduce some of the most important operators appearing in QED and establish some useful norm bounds on certain commutators involving them. These commutator estimates provide the main ingredients necessary to apply the general criterion of Section 2 to the QED models treated in this article. Their derivation is essentially based on the pull-through formula which is always employed either way to derive higher order estimates in quantum field theories [1, 2, 4, 5, 11]; compare Lemma 3.2 below. In Sections 4, 5, and 6 the general strategy from Section 2 is applied to the non- and semi-relativistic Pauli-Fierz operators and to the no-pair operator, respectively. The latter operators are introduced in detail in these sections. Apart from the fact that our estimate (1.2) is slightly stronger than the corresponding one of [4] the results of Sections 4 and 5 are not new and have been obtained earlier in [4]. However, in order to prove the higher order estimate (1.1) for the no-pair operator we virtually have to re-derive it for the semi-relativistic Pauli-Fierz operator by our own method anyway. Moreover, we think that the arguments employed in Sections 4 and 5 are more convenient and less involved than the procedure carried through in [4]. The main text is followed by an appendix where we show that the semi-relativistic Pauli-Fierz operator for a molecular system with static nuclei is semi-bounded below, provided that all Coulomb coupling constants are less than or equal to $2/\pi$. Moreover, we prove the same result for a molecular no-pair operator assuming that all Coulomb coupling constants are strictly less than the critical coupling constant of the Brown-Ravenhall model [3]. The results of the appendix are based on corresponding estimates for hydrogen-like atoms obtained in [10]. (We remark that the considerably stronger stability of matter of the second kind has been proven for a molecular no-pair operator in [9] under more restrictive assumptions on the involved physical parameters.) No restrictions on the values of the fine-structure constant or on the ultra-violet cut-off are imposed in the present article.

The main new results of this paper are Theorem 2.1 and its corollaries which provide general criteria for the validity of higher order estimates and Theorem 6.1 where higher order estimates for the no-pair operator are established.

Some frequently used notation. For $a, b \in \mathbb{R}$, we write $a \wedge b := \min\{a, b\}$ and $a \vee b := \max\{a, b\}$. $\mathcal{D}(T)$ denotes the domain of some operator T acting in some Hilbert space and $\mathcal{Q}(T)$ its form domain, when T is semi-bounded below. $C(a, b, \ldots), C'(a, b, \ldots)$, etc. denote constants that depend only on the quantities $a, b, \ldots$ and whose value might change from one estimate to another.

2. Higher order estimates: a general criterion

The following theorem and its succeeding corollaries present the key idea behind of our method. They essentially reduce the derivation of the higher order estimates to the verification of a certain sequence of form bounds. These form bounds can be verified easily without any further induction argument in the QED models treated in this paper.

Theorem 2.1. *Let H and F_ε, $\varepsilon > 0$, be self-adjoint operators in some Hilbert space $\mathscr{K}$ such that $H \geqslant 1$, $F_\varepsilon \geqslant 0$, and each F_ε is bounded. Let $m \in \mathbb{N} \cup \{\infty\}$, let $\mathscr{D}$ be a form core for H, and assume that the following conditions are fulfilled:*

(a) For every $\varepsilon > 0$, F_ε maps $\mathscr{D}$ into $\mathcal{Q}(H)$ and there is some $c_\varepsilon \in (0, \infty)$ such that

$$\big\langle F_\varepsilon \psi \,\big|\, H F_\varepsilon \psi \big\rangle \leqslant c_\varepsilon \langle \psi \,|\, H \psi \rangle, \qquad \psi \in \mathscr{D}.$$

(b) There is some $c \in [1, \infty)$ such that, for all $\varepsilon > 0$,

$$\langle \psi \,|\, F_\varepsilon^2 \psi \rangle \leqslant c^2 \langle \psi \,|\, H \psi \rangle, \qquad \psi \in \mathscr{D}.$$

(c) For every $n \in \mathbb{N}$, $n < m$, there is some $c_n \in [1, \infty)$ such that, for all $\varepsilon > 0$,

$$\begin{aligned} &\big| \langle H \varphi_1 \,|\, F_\varepsilon^n \varphi_2 \rangle - \langle F_\varepsilon^n \varphi_1 \,|\, H \varphi_2 \rangle \big| \\ &\quad \leqslant c_n \big\{ \langle \varphi_1 \,|\, H \varphi_1 \rangle + \langle F_\varepsilon^{n-1} \varphi_2 \,|\, H F_\varepsilon^{n-1} \varphi_2 \rangle \big\}, \qquad \varphi_1, \varphi_2 \in \mathscr{D}. \end{aligned}$$

Then it follows that, for every $n \in \mathbb{N}$, $n < m + 1$,

$$\| F_\varepsilon^n H^{-n/2} \| \leqslant C_n := 4^{n-1} c^n \prod_{\ell=1}^{n-1} c_\ell. \tag{2.1}$$

(An empty product equals 1 by definition.)

Proof. We define

$$T_\varepsilon(n) := H^{1/2} [F_\varepsilon^{n-1}, H^{-1}] H^{-(n-2)/2}, \qquad n \in \{2, 3, 4, \ldots\}.$$

$T_\varepsilon(n)$ is well-defined and bounded because of the closed graph theorem and Condition (a), which implies that $F_\varepsilon \in \mathscr{L}(\mathcal{Q}(H))$, where $\mathcal{Q}(H) = \mathcal{D}(H^{1/2})$

is equipped with the form norm. We shall prove the following sequence of assertions by induction on $n \in \mathbb{N}$, $n < m+1$.

$$A(n) \;:\Leftrightarrow \quad \text{The bound (2.1) holds true and, if } n>3, \text{ we have}$$

$$\forall\,\varepsilon>0\;:\quad \|T_\varepsilon(n)\|\,\leqslant\,C_n/4c^2\,. \tag{2.2}$$

For $n=1$, the bound (2.1) is fulfilled with $C_1=c$ on account of Condition (b). Next, assume that $n\in\mathbb{N}$, $n<m$, and that $A(1),\ldots,A(n)$ hold true. To find a bound on $\|F_\varepsilon^{n+1}\,H^{-(n+1)/2}\|$ we write

$$F_\varepsilon^{n+1}\,H^{-(n+1)/2}\;=\;Q_1\,+\,Q_2 \tag{2.3}$$

with

$$Q_1\;:=\;F_\varepsilon\,H^{-1}\,F_\varepsilon^n\,H^{-(n-1)/2}\,,\qquad Q_2\;:=\;F_\varepsilon\,\big[\,F_\varepsilon^n\,,\,H^{-1}\,\big]\,H^{-(n-1)/2}\,.$$

By the induction hypothesis we have

$$\|Q_1\|\leqslant\|F_\varepsilon\,H^{-1/2}\|\,\|H^{-1/2}\,F_\varepsilon\,\|\,\|F_\varepsilon^{n-1}\,H^{-(n-1)/2}\|\leqslant c^2\,C_{n-1}\,, \tag{2.4}$$

where $C_0:=1$. Moreover, we observe that

$$\|Q_2\|\;=\;\|F_\varepsilon\,H^{-1/2}\,T_\varepsilon(n+1)\|\;\leqslant\;c\,\|T_\varepsilon(n+1)\|\,. \tag{2.5}$$

To find a bound on $\|T_\varepsilon(n+1)\|$ we recall that F_ε maps the form domain of H continuously into itself. In particular, since $\mathscr{D}$ is a form core for H the form bound appearing in Condition (c) is available, for all $\varphi_1,\varphi_2\in\mathcal{Q}(H)$. Let $\phi,\psi\in\mathscr{D}$. Applying Condition (c), extended in this way, with

$$\varphi_1\;=\;\delta^{1/2}\,H^{-1/2}\,\phi\in\mathcal{Q}(H)\,,\qquad \varphi_2\;=\;\delta^{-1/2}\,H^{-(n+1)/2}\,\psi\in\mathcal{Q}(H)\,,$$

for some $\delta>0$, we obtain

$$\begin{aligned}
&|\langle\,\phi\,|\,T_\varepsilon(n+1)\,\psi\,\rangle|\\
&\quad=\;\big|\big\langle\,H\,H^{-1/2}\,\phi\,\big|\,F_\varepsilon^n\,H^{-(n+1)/2}\,\psi\,\big\rangle-\big\langle\,F_\varepsilon^n\,H^{-1/2}\,\phi\,\big|\,H\,H^{-(n+1)/2}\,\psi\,\big\rangle\big|\\
&\quad\leqslant\;c_n\,\inf_{\delta>0}\big\{\,\delta\,\|\phi\|^2+\delta^{-1}\,\|\{H^{1/2}\,F_\varepsilon^{n-1}\,H^{-n/2}\}\,H^{-1/2}\,\psi\|^2\,\big\}\\
&\quad\leqslant\;2\,c_n\,\|\{H^{1/2}\,F_\varepsilon^{n-1}\,H^{-n/2}\}\|\,\|\phi\|\,\|\psi\|\,.
\end{aligned}$$

The operator $\{\cdots\}$ is just the identity when $n=1$. For $n>1$, it can be written as

$$H^{1/2}\,F_\varepsilon^{n-1}\,H^{-n/2}\;=\;\{H^{-1/2}\,F_\varepsilon\}\,F_\varepsilon^{n-2}\,H^{-(n-2)/2}\;+\;T_\varepsilon(n)\,. \tag{2.6}$$

Applying the induction hypothesis and $c,c_\ell\geqslant 1$, we thus get $\|T_\varepsilon(2)\|\leqslant 2\,c_1$, $\|T_\varepsilon(3)\|\leqslant 6\,c\,c_1c_2$, $\|T_\varepsilon(4)\|\leqslant 14\,c^2c_1c_2c_3<C_4/4c^2$, and

$$\begin{aligned}
c\,\|T_\varepsilon(n+1)\|\;&=\;c\,\sup\big\{\,|\langle\,\phi\,|\,T_\varepsilon(n+1)\,\psi\,\rangle|\;:\;\phi,\psi\in\mathscr{D}\,,\;\|\phi\|=\|\psi\|=1\,\big\}\\
&\leqslant\;2\,c_n\,(c^2\,C_{n-2}+C_n/4c)\;<\;c_n\,C_n\;=\;C_{n+1}/4c\,,\qquad n>3\,,
\end{aligned}$$

since $c^2\,C_{n-2}\leqslant C_n/16$, for $n>3$. Taking (2.3)–(2.5) into account we arrive at $\|F_\varepsilon^2\,H^{-1}\|\leqslant c^2+2c\,c_1<C_2$, $\|F_\varepsilon^3\,H^{-3/2}\|\leqslant c^3+6c^2c_1c_2<C_3$, and

$$\|F_\varepsilon^{n+1}\,H^{-(n+1)/2}\|\;<\;c^2\,C_{n-2}+C_{n+1}/4c\;<\;C_{n+1}\,,\qquad n>3\,,$$

which concludes the induction step. □

Corollary 2.2. *Assume that H and F_ε, $\varepsilon > 0$, are self-adjoint operators in some Hilbert space $\mathscr{K}$ that fulfill the assumptions of Theorem 2.1 with (c) replaced by the stronger condition*

(c') For every $n \in \mathbb{N}$, $n < m$, there is some $c_n \in [1,\infty)$ such that, for all $\varepsilon > 0$,

$$\begin{aligned}&\big|\langle H\varphi_1 \,|\, F_\varepsilon^n \varphi_2\rangle - \langle F_\varepsilon^n \varphi_1 \,|\, H\varphi_2\rangle\big|\\ &\quad\leqslant c_n\big\{\|\varphi_1\|^2 + \langle F_\varepsilon^{n-1}\varphi_2 \,|\, H F_\varepsilon^{n-1}\varphi_2\rangle\big\}, \qquad \varphi_1,\varphi_2 \in \mathscr{D}.\end{aligned}$$

Then, in addition to (2.1), it follows that, for $n \in \mathbb{N}$, $n < m$, $[F_\varepsilon^n, H]\,H^{-n/2}$ defines a bounded sesquilinear form with domain $\mathcal{Q}(H)\times\mathcal{Q}(H)$ and

$$\big\|\,[F_\varepsilon^n, H]\,H^{-n/2}\,\big\| \leqslant C_n' := 4^n\,c^{n-1}\prod_{\ell=1}^n c_\ell\,. \tag{2.7}$$

Proof. Again, the form bound in (c') is available, for all $\varphi_1,\varphi_2\in\mathcal{Q}(H)$, whence

$$\begin{aligned}&\big|\langle H\phi \,|\, F_\varepsilon^n H^{-n/2}\psi\rangle - \langle F_\varepsilon^n\phi \,|\, H H^{-n/2}\psi\rangle\big|\\ &\leqslant c_n \inf_{\delta>0}\big\{\delta\|\phi\|^2 + \delta^{-1}\big\|H^{1/2}F_\varepsilon^{n-1}H^{-n/2}\psi\big\|^2\big\} \leqslant 2\,c_n\,\|H^{1/2}F_\varepsilon^{n-1}H^{-n/2}\|\,,\end{aligned}$$

for all normalized $\phi,\psi\in\mathcal{Q}(H)$. The assertion now follows from (2.1), (2.6), and the bounds on $\|T_\varepsilon(n)\|$ given in the proof of Theorem 2.1. □

Corollary 2.3. *Let $H \geqslant 1$ and $A \geqslant 0$ be two self-adjoint operators in some Hilbert space $\mathscr{K}$. Let $\kappa > 0$, define*

$$f_\varepsilon(t) := t/(1+\varepsilon t)\,, \quad t\geqslant 0\,, \qquad F_\varepsilon := f_\varepsilon^\kappa(A)\,,$$

for all $\varepsilon > 0$, and assume that H and F_ε, $\varepsilon > 0$, fulfill the hypotheses of Theorem 2.1, for some $m \in \mathbb{N}\cup\{\infty\}$. Then $\mathrm{Ran}(H^{-n/2}) \subset \mathcal{D}(A^{\kappa n})$, for every $n\in\mathbb{N}$, $n < m+1$, and

$$\big\|\,A^{\kappa n}H^{-n/2}\,\big\| \leqslant 4^{n-1}\,c^n\prod_{\ell=1}^{n-1}c_\ell\,.$$

If H and F_ε, $\varepsilon > 0$, fulfill the hypotheses of Corollary 2.2, then, for every $n \in\mathbb{N}$, $n<m$, it additionally follows that $A^{\kappa n}H^{-n/2}$ maps $\mathcal{D}(H)$ into itself so that $[A^{\kappa n}, H]\,H^{-n/2}$ is well-defined on $\mathcal{D}(H)$, and

$$\big\|\,[A^{\kappa n}, H]\,H^{-n/2}\,\big\| \leqslant 4^n\,c^{n-1}\prod_{\ell=1}^n c_\ell\,.$$

Proof. Let $U : \mathscr{K} \to L^2(\Omega,\mu)$ be a unitary transformation such that $a = U\,A\,U^*$ is a maximal operator of multiplication with some non-negative measurable function – again called a – on some measure space $(\Omega,\mathfrak{A},\mu)$. We pick some $\psi\in\mathscr{K}$, set $\phi_n := U\,H^{-n/2}\psi$, and apply the monotone convergence theorem to conclude that

$$\int_\Omega a(\omega)^{2\kappa\, n}\,|\phi_n(\omega)|^2\,d\mu(\omega) \;=\; \lim_{\varepsilon\searrow 0}\int_\Omega f_\varepsilon^\kappa(a(\omega))^{2n}\,|\phi_n(\omega)|^2\,d\mu(\omega)$$
$$= \lim_{\varepsilon\searrow 0}\|F_\varepsilon^n\,H^{-n/2}\,\psi\|^2 \;\leqslant\; C_n\,\|\psi\|^2,$$

for every $n\in\mathbb{N}$, $n<m+1$, which implies the first assertion. Now, assume that H and F_ε, $\varepsilon>0$, fulfill Condition (c') of Corollary 2.2. Applying the dominated convergence theorem in the spectral representation introduced above we see that $F_\varepsilon^n\,\psi\to A^{\kappa\, n}\,\psi$, for every $\psi\in\mathcal{D}(A^{\kappa\, n})$. Hence, (2.7) and $\mathrm{Ran}(H^{-n/2})\subset\mathcal{D}(A^{\kappa\, n})$ imply, for $n<m$ and $\phi,\psi\in\mathcal{D}(H)$,

$$\big|\big\langle\,\phi\,\big|\,A^{\kappa\, n}H^{-n/2}\,H\,\psi\,\big\rangle-\big\langle\,H\,\phi\,\big|\,A^{\kappa\, n}\,H^{-n/2}\,\psi\,\big\rangle\big|$$
$$=\lim_{\varepsilon\searrow 0}\big|\big\langle\,F_\varepsilon^n\,\phi\,\big|\,H\,H^{-n/2}\,\psi\,\big\rangle-\big\langle\,H\,\phi\,\big|\,F_\varepsilon^n\,H^{-n/2}\,\psi\,\big\rangle\big|$$
$$\leqslant\limsup_{\varepsilon\searrow 0}\big\|\,[F_\varepsilon^n\,,\,H]\,H^{-n/2}\,\big\|\,\|\phi\|\,\|\psi\|\;\leqslant\;C_n'\,\|\phi\|\,\|\psi\|\,.$$

Thus, $|\langle\,H\,\phi\,|\,A^{\kappa\, n}\,H^{-n/2}\,\psi\,\rangle|\leqslant\|\phi\|\,\|A^{\kappa\, n}\,H^{-n/2}\|\,\|H\,\psi\|+C_n'\|\phi\|\,\|\psi\|$, for all $\phi,\psi\in\mathcal{D}(H)$. In particular, $A^{\kappa\, n}\,H^{-n/2}\,\psi\in\mathcal{D}(H^*)=\mathcal{D}(H)$, for all $\psi\in\mathcal{D}(H)$, and the second asserted bound holds true. □

3. Commutator estimates

In this section we derive operator norm bounds on commutators involving the quantized vector potential, $\mathbf{A}$, the radiation field energy, H_{f}, and the Dirac operator, $D_{\mathbf{A}}$. The underlying Hilbert space is

$$\mathscr{H}\;:=\;L^2(\mathbb{R}^3_{\mathbf{x}}\times\mathbb{Z}_4)\otimes\mathscr{F}_{\mathrm{b}}\;=\;\int_{\mathbb{R}^3}^{\oplus}\mathbb{C}^4\otimes\mathscr{F}_{\mathrm{b}}\,d^3\mathbf{x}\,,$$

where the bosonic Fock space, $\mathscr{F}_{\mathrm{b}}$, is modeled over the one-photon Hilbert space

$$\mathscr{F}_{\mathrm{b}}^{(1)}\;:=\;L^2(\mathcal{A}\times\mathbb{Z}_2,dk)\,,\qquad\int dk\;:=\;\sum_{\lambda\in\mathbb{Z}_2}\int_{\mathcal{A}}d^3\mathbf{k}\,.$$

With regards to the applications in [8] we define $\mathcal{A}:=\{\mathbf{k}\in\mathbb{R}^3:\,|\mathbf{k}|\geqslant m\}$, for some $m\geqslant 0$. We thus have

$$\mathscr{F}_{\mathrm{b}}=\bigoplus_{n=0}^{\infty}\mathscr{F}_{\mathrm{b}}^{(n)},\qquad\mathscr{F}_{\mathrm{b}}^{(0)}:=\mathbb{C}\,,\quad\mathscr{F}_{\mathrm{b}}^{(n)}:=\mathcal{S}_n\,L^2\big((\mathcal{A}\times\mathbb{Z}_2)^n\big),\;n\in\mathbb{N},$$

where $\mathcal{S}_n=\mathcal{S}_n^2=\mathcal{S}_n^*$ is given by

$$(\mathcal{S}_n\,\psi^{(n)})(k_1,\dots,k_n):=\frac{1}{n!}\sum_{\pi\in\mathfrak{S}_n}\psi^{(n)}(k_{\pi(1)},\dots,k_{\pi(n)}),$$

for every $\psi^{(n)}\in L^2\big((\mathcal{A}\times\mathbb{Z}_2)^n\big)$, $\mathfrak{S}_n$ denoting the group of permutations of $\{1,\dots,n\}$. The vector potential is determined by a certain vector-valued function, $\mathbf{G}$, called the form factor.

Hypothesis 3.1. *The dispersion relation,* $\omega : \mathcal{A} \to [0,\infty)$*, is a measurable function such that* $0 < \omega(k) := \omega(\mathbf{k}) \leqslant |\mathbf{k}|$*, for* $k = (\mathbf{k},\lambda) \in \mathcal{A}\times\mathbb{Z}_2$ *with* $\mathbf{k} \neq 0$*. For every* $k \in (\mathcal{A}\backslash\{0\})\times\mathbb{Z}_2$ *and* $j \in \{1,2,3\}$*,* $G^{(j)}(k)$ *is a bounded continuously differentiable function,* $\mathbb{R}^3_{\mathbf{x}} \ni \mathbf{x} \mapsto G^{(j)}_{\mathbf{x}}(k)$*, such that the map* $(\mathbf{x},k) \mapsto G^{(j)}_{\mathbf{x}}(k)$ *is measurable and* $G^{(j)}_{\mathbf{x}}(-\mathbf{k},\lambda) = \overline{G^{(j)}_{\mathbf{x}}(\mathbf{k},\lambda)}$*, for almost every* $\mathbf{k}$ *and all* $\mathbf{x} \in \mathbb{R}^3$ *and* $\lambda \in \mathbb{Z}_2$*. Finally, there exist* $d_{-1}, d_0, d_1, \ldots \in (0,\infty)$ *such that*

$$2\int \omega(k)^{\ell}\,\|\mathbf{G}(k)\|^2_\infty\,dk \;\leqslant\; d_\ell^2\,, \qquad \ell \in \{-1,0,1,2,\ldots\}\,, \tag{3.1}$$

$$2\int \omega(k)^{-1}\,\|\nabla_{\mathbf{x}}\wedge\mathbf{G}(k)\|^2_\infty\,dk \;\leqslant\; d_1^2\,, \tag{3.2}$$

where $\mathbf{G} = (G^{(1)},G^{(2)},G^{(3)})$ *and* $\|\mathbf{G}(k)\|_\infty := \sup_{\mathbf{x}}|\mathbf{G}_{\mathbf{x}}(k)|$*, etc.*

Example. In the physical applications the form factor is often given as

$$\mathbf{G}^{e,\Lambda}_{\mathbf{x}}(k) \;:=\; -e\,\frac{\mathbb{1}_{\{|\mathbf{k}|\leqslant\Lambda\}}}{2\pi\sqrt{|\mathbf{k}|}}\,e^{-i\mathbf{k}\cdot\mathbf{x}}\,\boldsymbol{\varepsilon}(k), \tag{3.3}$$

for $(\mathbf{x},k) \in \mathbb{R}^3\times(\mathbb{R}^3\times\mathbb{Z}_2)$ with $\mathbf{k}\neq 0$. Here the physical units are chosen such that energies are measured in units of the rest energy of the electron. Length are measured in units of one Compton wave length divided by 2π. The parameter $\Lambda > 0$ is an ultraviolet cut-off and the square of the elementary charge, $e > 0$, equals Sommerfeld's fine-structure constant in these units; we have $e^2 \approx 1/137$ in nature. The polarization vectors, $\boldsymbol{\varepsilon}(\mathbf{k},\lambda)$, $\lambda\in\mathbb{Z}_2$, are homogeneous of degree zero in $\mathbf{k}$ such that $\{\mathring{\mathbf{k}}, \boldsymbol{\varepsilon}(\mathring{\mathbf{k}},0), \boldsymbol{\varepsilon}(\mathring{\mathbf{k}},1)\}$ is an orthonormal basis of $\mathbb{R}^3$, for every $\mathring{\mathbf{k}} \in S^2$. This corresponds to the Coulomb gauge for $\nabla_{\mathbf{x}}\cdot\mathbf{G}^{e,\Lambda} = 0$. We remark that the vector fields $S^2 \ni \mathring{\mathbf{k}} \mapsto \boldsymbol{\varepsilon}(\mathring{\mathbf{k}},\lambda)$ are necessarily discontinuous. ⋄

It is useful to work with more general form factors fulfilling Hypothesis 3.1 since in the study of the existence of ground states in QED one usually encounters truncated and discretized versions of the physical choice $\mathbf{G}^{e,\Lambda}$. For the applications in [8] it is necessary to know that the higher order estimates established here hold true uniformly in the involved parameters and Hypothesis 3.1 is convenient way to handle this.
We recall the definition of the creation and the annihilation operators of a photon state $f \in \mathscr{F}_{\mathrm{b}}^{(1)}$,

$$(a^\dagger(f)\,\psi)^{(n)}(k_1,\ldots,k_n) = n^{-1/2}\sum_{j=1}^{n} f(k_j)\,\psi^{(n-1)}(\ldots,k_{j-1},k_{j+1},\ldots),\;\; n\in\mathbb{N},$$

$$(a(f)\,\psi)^{(n)}(k_1,\ldots,k_n) = (n+1)^{1/2}\int \overline{f}(k)\,\psi^{(n+1)}(k,k_1,\ldots,k_n)\,dk,\;\; n\in\mathbb{N}_0,$$

and $(a^\dagger(f)\,\psi)^{(0)} = 0$, $a(f)\,(\psi^{(0)},0,0,\ldots) = 0$, for all $\psi = (\psi^{(n)})_{n=0}^\infty \in \mathscr{F}_{\mathrm{b}}$ such that the right hand sides again define elements of $\mathscr{F}_{\mathrm{b}}$. $a^\dagger(f)$ and $a(f)$ are formal adjoints of each other on the dense domain

$$\mathscr{C}_0 := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathcal{S}_n \, L^\infty_{\mathrm{comp}}\big((\mathcal{A}\times\mathbb{Z}_2)^n\big) . \qquad \text{(Algebraic direct sum.)}$$

For a three-vector of functions $\mathbf{f} = (f^{(1)}, f^{(2)}, f^{(3)}) \in (\mathscr{F}_{\mathrm{b}}^{(1)})^3$, we write $a^\sharp(\mathbf{f}) := (a^\sharp(f^{(1)}), a^\sharp(f^{(2)}), a^\sharp(f^{(3)}))$, where $a^\sharp$ is $a^\dagger$ or a. Then the quantized vector potential is the triplet of operators given by

$$\mathbf{A} \equiv \mathbf{A}(\mathbf{G}) := a^\dagger(\mathbf{G}) + a(\mathbf{G}) , \qquad a^\sharp(\mathbf{G}) := \int_{\mathbb{R}^3}^{\oplus} \mathbb{1}_{\mathbb{C}^4} \otimes a^\sharp(\mathbf{G}_{\mathbf{x}}) \, d^3\mathbf{x} .$$

The radiation field energy is the direct sum $H_{\mathrm{f}} = \bigoplus_{n=0}^{\infty} d\Gamma^{(n)}(\omega) : \mathcal{D}(H_{\mathrm{f}}) \subset \mathscr{F}_{\mathrm{b}} \to \mathscr{F}_{\mathrm{b}}$, where $d\Gamma^{(0)}(\omega) := 0$, and $d\Gamma^{(n)}(\omega)$ denotes the maximal multiplication operator in $\mathscr{F}_{\mathrm{b}}^{(n)}$ associated with the symmetric function $(k_1, \ldots, k_n) \mapsto \omega(k_1) + \cdots + \omega(k_n)$. By the permutation symmetry and Fubini's theorem we thus have

$$\big\langle H_{\mathrm{f}}^{1/2} \phi \,\big|\, H_{\mathrm{f}}^{1/2} \psi \big\rangle = \int \omega(k) \, \langle a(k)\,\phi \,|\, a(k)\,\psi \rangle \, dk , \qquad \phi, \psi \in \mathcal{D}(H_{\mathrm{f}}^{1/2}) , \tag{3.4}$$

where we use the notation

$$(a(k)\,\psi)^{(n)}(k_1, \ldots, k_n) = (n+1)^{1/2} \, \psi^{(n+1)}(k, k_1, \ldots, k_n) , \quad n \in \mathbb{N}_0 ,$$

almost everywhere, and $a(k)\,(\psi^{(0)}, 0, 0, \ldots) = 0$. For a measurable function $f : \mathbb{R} \to \mathbb{R}$ and $\psi \in \mathcal{D}(f(H_{\mathrm{f}}))$, the following identity in $\mathscr{F}_{\mathrm{b}}^{(n)}$,

$$(a(k)\, f(H_{\mathrm{f}})\, \psi)^{(n)} = f\big(\omega(k) + d\Gamma^{(n)}(\omega)\big)\, (a(k)\,\psi)^{(n)} , \qquad n \in \mathbb{N}_0 ,$$

valid for almost every k, is called the pull-through formula. Finally, we let $\alpha_1, \alpha_2, \alpha_3$, and $\beta := \alpha_0$ denote hermitian four times four matrices that fulfill the Clifford algebra relations

$$\alpha_i \, \alpha_j + \alpha_j \, \alpha_i = 2 \, \delta_{ij} \, \mathbb{1} , \qquad i, j \in \{0, 1, 2, 3\} . \tag{3.5}$$

They act on the second tensor factor in $L^2(\mathbb{R}^3_{\mathbf{x}} \times \mathbb{Z}_4) = L^2(\mathbb{R}^3_{\mathbf{x}}) \otimes \mathbb{C}^4$. As a consequence of (3.5) and the C^*-equality we have

$$\|\boldsymbol{\alpha} \cdot \mathbf{v}\|_{\mathscr{L}(\mathbb{C}^4)} = |\mathbf{v}| , \quad \mathbf{v} \in \mathbb{R}^3 , \qquad \|\boldsymbol{\alpha} \cdot \mathbf{z}\|_{\mathscr{L}(\mathbb{C}^4)} \leqslant \sqrt{2}\, |\mathbf{z}| , \quad \mathbf{z} \in \mathbb{C}^3 , \tag{3.6}$$

where $\boldsymbol{\alpha} \cdot \mathbf{z} := \alpha_1 \, z^{(1)} + \alpha_2 \, z^{(2)} + \alpha_3 \, z^{(3)}$, for $\mathbf{z} = (z^{(1)}, z^{(2)}, z^{(3)}) \in \mathbb{C}^3$. A standard exercise using the inequality in (3.6), the Cauchy-Schwarz inequality, and the canonical commutation relations,

$$[a^\sharp(f) \,,\, a^\sharp(g)] = 0 , \qquad [a(f) \,,\, a^\dagger(g)] = \langle f \,|\, g \rangle \, \mathbb{1} , \qquad f, g \in \mathscr{F}_{\mathrm{b}}^{(1)} ,$$

reveals that every $\psi \in \mathcal{D}(H_{\mathrm{f}}^{1/2})$ belongs to the domain of $\boldsymbol{\alpha} \cdot a^\sharp(\mathbf{G})$ and

$$\|\boldsymbol{\alpha} \cdot a(\mathbf{G})\, \psi\| \leqslant d_{-1} \, \|H_{\mathrm{f}}^{1/2} \, \psi\| , \quad \|\boldsymbol{\alpha} \cdot a^\dagger(\mathbf{G})\, \psi\|^2 \leqslant d_{-1}^2 \, \|H_{\mathrm{f}}^{1/2} \, \psi\|^2 + d_0^2 \, \|\psi\|^2. \tag{3.7}$$

(Here and in the following we identify $H_{\mathrm{f}} \equiv \mathbb{1} \otimes H_{\mathrm{f}}$, etc.) These relative bounds imply that $\boldsymbol{\alpha} \cdot \mathbf{A}$ is symmetric on the domain $\mathcal{D}(H_{\mathrm{f}}^{1/2})$.

The operators whose norms are estimated in (3.9) and the following lemmata are always well-defined a priori on the following dense subspace of $\mathscr{H}$,

$$\mathscr{D} := C_0^\infty(\mathbb{R}^3 \times \mathbb{Z}_4) \otimes \mathscr{C}_0 . \qquad \text{(Algebraic tensor product.)}$$

Given some $E \geqslant 1$ we set

$$\check{H}_{\mathrm{f}} := H_{\mathrm{f}} + E \tag{3.8}$$

in the sequel. We already know from [10] that, for every $\nu \geqslant 0$, there is some constant, $C_\nu \in (0,\infty)$, such that

$$\big\| \, [\boldsymbol{\alpha} \cdot \mathbf{A} \, , \, \check{H}_{\mathrm{f}}^{-\nu}] \, \check{H}_{\mathrm{f}}^{\nu} \, \big\| \leqslant C_\nu / E^{1/2} \, , \qquad E \geqslant 1 \, . \tag{3.9}$$

In our first lemma we derive a generalization of (3.9). Its proof resembles the one of (3.9) given in [10]. Since we shall encounter many similar but slightly different commutators in the applications it makes sense to introduce the numerous parameters that obscure its statement (but simplify its proof).

Lemma 3.2. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1. Let $\varepsilon \geqslant 0$, $E \geqslant 1$, $\kappa, \nu \in \mathbb{R}$, $\gamma, \delta, \sigma, \tau \geqslant 0$, such that $\gamma + \delta + \sigma + \tau \leqslant 1/2$, and define*

$$f_\varepsilon(t) := \frac{t + E}{1 + \varepsilon t + \varepsilon E} \, , \qquad t \in [0, \infty) \, . \tag{3.10}$$

Then the operator $\check{H}_{\mathrm{f}}^{\nu+\gamma} \, f_\varepsilon^{\sigma}(H_{\mathrm{f}}) \, [\boldsymbol{\alpha} \cdot \mathbf{A} \, , \, f_\varepsilon^{\kappa}(H_{\mathrm{f}})] \, \check{H}_{\mathrm{f}}^{-\nu+\delta} f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})$, defined a priori on $\mathscr{D}$, extends to a bounded operator on $\mathscr{H}$ and

$$\begin{aligned} &\big\| \, \check{H}_{\mathrm{f}}^{\nu+\gamma} \, f_\varepsilon^{\sigma}(H_{\mathrm{f}}) \, [\boldsymbol{\alpha} \cdot \mathbf{A} \, , \, f_\varepsilon^{\kappa}(H_{\mathrm{f}})] \, \check{H}_{\mathrm{f}}^{-\nu+\delta} \, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}}) \, \big\| \\ &\qquad \leqslant |\kappa| \, 2^{(\rho+1)/2} \, (d_1 + d_\rho) \, E^{\gamma+\delta+\sigma+\tau-1/2} \, , \end{aligned} \tag{3.11}$$

where ρ is the smallest integer greater or equal to $3 + 2|\kappa| + 2|\nu|$.

Proof. We notice that all operators $\check{H}_{\mathrm{f}}^{s}$ and $f_\varepsilon^{s}(H_{\mathrm{f}})$ leave the dense subspace $\mathscr{D}$ invariant and that $\boldsymbol{\alpha} \cdot a^\sharp(\mathbf{G})$ maps $\mathscr{D}$ into $\mathcal{D}(\check{H}_{\mathrm{f}}^{s})$, for every $s \in \mathbb{R}$. Now, let $\varphi, \psi \in \mathscr{D}$. Then

$$\big\langle \, \varphi \, \big| \, \check{H}_{\mathrm{f}}^{\nu+\gamma} \, f_\varepsilon^{\sigma}(H_{\mathrm{f}}) \, [\boldsymbol{\alpha} \cdot \mathbf{A} \, , \, f_\varepsilon^{\kappa}(H_{\mathrm{f}})] \, \check{H}_{\mathrm{f}}^{-\nu+\delta} \, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}}) \, \psi \, \big\rangle$$

$$= \big\langle \, \varphi \, \big| \, \check{H}_{\mathrm{f}}^{\nu+\gamma} \, f_\varepsilon^{\sigma}(H_{\mathrm{f}}) \, [\boldsymbol{\alpha} \cdot a(\mathbf{G}) \, , \, f_\varepsilon^{\kappa}(H_{\mathrm{f}})] \, \check{H}_{\mathrm{f}}^{-\nu+\delta} \, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}}) \, \psi \, \big\rangle \tag{3.12}$$

$$- \big\langle \, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}}) \, \check{H}_{\mathrm{f}}^{-\nu+\delta} \, [\boldsymbol{\alpha} \cdot a(\mathbf{G}) \, , \, f_\varepsilon^{\kappa}(H_{\mathrm{f}})] \, f_\varepsilon^{\sigma}(H_{\mathrm{f}}) \, \check{H}_{\mathrm{f}}^{\nu+\gamma} \, \varphi \, \big| \, \psi \, \big\rangle \, . \tag{3.13}$$

For almost every k, the pull-through formula yields the following representation,

$$\check{H}_{\mathrm{f}}^{\nu+\gamma} \, f_\varepsilon^{\sigma}(H_{\mathrm{f}}) \, [a(k) \, , \, f_\varepsilon^{\kappa}(H_{\mathrm{f}})] \, \check{H}_{\mathrm{f}}^{-\nu+\delta} \, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}}) \, \psi = F(k; H_{\mathrm{f}}) \, a(k) \, \check{H}_{\mathrm{f}}^{-1/2} \, \psi \, ,$$

where

$$\begin{aligned} F(k;t) \,:=\, & (t+E)^{\nu+\gamma}\, f_\varepsilon^\sigma(t)\,\big(f_\varepsilon^\kappa(t+\omega(k))-f_\varepsilon^\kappa(t)\big) \\ & \cdot (t+E+\omega(k))^{-\nu+\delta+1/2}\, f_\varepsilon^{-\kappa+\tau}(t+\omega(k)) \\ =\, & \Big(\frac{t+E}{t+E+\omega(k)}\Big)^\nu (t+E)^\gamma\,(t+E+\omega(k))^{\delta+1/2} \\ & \cdot \int_0^1 \frac{d}{ds} f_\varepsilon^\kappa(t+s\,\omega(k))\,ds\, \frac{f_\varepsilon^\sigma(t)\, f_\varepsilon^\tau(t+\omega(k))}{f_\varepsilon^\kappa(t+\omega(k))}\,, \end{aligned}$$

for $t \geqslant 0$. We compute

$$\frac{d}{ds} f_\varepsilon^\kappa(t+s\,\omega(k)) \,=\, \frac{\kappa\,\omega(k)\, f_\varepsilon^\kappa(t+s\,\omega(k))}{(t+s\,\omega(k)+E)(1+\varepsilon\,t+\varepsilon\,s\,\omega(k)+\varepsilon\,E)}\,. \tag{3.14}$$

Using that f_ε is increasing in $t \geqslant 0$ and that

$$(t+\omega(k)+E)/(t+s\,\omega(k)+E) \,\leqslant\, 1+\omega(k)\,, \qquad s\in[0,1]\,,$$

thus

$$f_\varepsilon^\kappa(t+s\,\omega(k))/f_\varepsilon^\kappa(t+\omega(k)) \,\leqslant\, (1+\omega(k))^{-(0\wedge\kappa)}\,, \qquad s\in[0,1]\,,$$

it is elementary to verify that

$$|F_\varepsilon(k;t)| \,\leqslant\, |\kappa|\,\omega(k)\,(1+\omega(k))^{\delta+\tau-(0\wedge\kappa)-(0\wedge\nu)+1/2}\, E^{\gamma+\delta+\sigma+\tau-1/2}\,,$$

for all $t \geqslant 0$ and k. We deduce that the term in (3.12) can be estimated as

$$\begin{aligned} & \big|\big\langle\,\varphi\,\big|\, \check{H}_{\mathrm{f}}^{\nu+\gamma}\, f_\varepsilon^\sigma(H_{\mathrm{f}})\,[\boldsymbol{\alpha}\cdot a(\mathbf{G})\,,\, f_\varepsilon^\kappa(H_{\mathrm{f}})]\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\psi\,\big\rangle\big| \\ & \leqslant \int \|\varphi\|\,\big\|\boldsymbol{\alpha}\cdot\mathbf{G}(k)\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\, f_\varepsilon^\sigma(H_{\mathrm{f}})\,[a(k)\,,\, f_\varepsilon^\kappa(H_{\mathrm{f}})]\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\, f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\psi\big\|\,dk \\ & \leqslant \sqrt{2}\int \|\varphi\|\,\|\mathbf{G}(k)\|_\infty\,\|F_\varepsilon(k;H_{\mathrm{f}})\|\,\|a(k)\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\|\,dk \\ & \leqslant |\kappa|\,\sqrt{2}\Big(\int \omega(k)\,(1+\omega(k))^{2(\delta+\tau)-(0\wedge 2\kappa)-(0\wedge 2\nu)+1}\,\|\mathbf{G}(k)\|_\infty^2\,dk\Big)^{1/2} \\ & \qquad \cdot \Big(\int \omega(k)\,\big\|\,a(k)\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\big\|^2\,dk\Big)^{1/2}\,\|\varphi\|\,E^{\gamma+\delta+\sigma+\tau-1/2} \\ & \leqslant\, |\kappa|\,2^{(\rho-1)/2}\,(d_1+d_\rho)\,\|\varphi\|\,\big\|\,H_{\mathrm{f}}^{1/2}\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\big\|\,E^{\gamma+\delta+\sigma+\tau-1/2}\,. \end{aligned} \tag{3.15}$$

In the last step we used $\delta+\tau \leqslant 1/2$ and applied (3.4). (3.15) immediately gives a bound on the term in (3.13), too. For we have

$$\begin{aligned} & f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\,[\boldsymbol{\alpha}\cdot a(\mathbf{G})\,,\, f_\varepsilon^\kappa(H_{\mathrm{f}})]\, f_\varepsilon^\sigma(H_{\mathrm{f}})\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\,\varphi \\ & \qquad = \check{H}_{\mathrm{f}}^{-\nu+\delta}\, f_\varepsilon^\tau(H_{\mathrm{f}})\,[f_\varepsilon^{-\kappa}(H_{\mathrm{f}})\,,\,\boldsymbol{\alpha}\cdot a(\mathbf{G})]\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\, f_\varepsilon^{\kappa+\sigma}(H_{\mathrm{f}})\,\varphi\,, \end{aligned}$$

which after the replacements $(\nu,\kappa,\gamma,\delta,\sigma,\tau)\mapsto(-\nu,-\kappa,\delta,\gamma,\tau,\sigma)$ and $\varphi\mapsto-\psi$ is precisely the term we just have treated. □

Lemma 3.2 provides all the information needed to apply Corollary 2.3 to non-relativistic QED. For the application of Corollary 2.3 to the non-local semi-relativistic models of QED it is necessary to study commutators that involve resolvents and sign functions of the Dirac operator,

$$D_{\mathbf{A}} := \boldsymbol{\alpha} \cdot (-i\nabla_{\mathbf{x}} + \mathbf{A}) + \beta .$$

An application of Nelson's commutator theorem with test operator $-\Delta + H_f + 1$ shows that $D_{\mathbf{A}}$ is essentially self-adjoint on $\mathscr{D}$. The spectrum of its unique closed extension, again denoted by the same symbol, is contained in the union of two half-lines, $\sigma[D_{\mathbf{A}}] \subset (-\infty, -1] \cup [1, \infty)$. In particular, it makes sense to define

$$R_{\mathbf{A}}(iy) := (D_{\mathbf{A}} - iy)^{-1} , \qquad y \in \mathbb{R} ,$$

and the spectral calculus yields

$$\|R_{\mathbf{A}}(iy)\| \leqslant (1+y^2)^{-1/2}, \qquad \int_{\mathbb{R}} \big\| \, |D_{\mathbf{A}}|^{1/2} \, R_{\mathbf{A}}(iy) \, \psi \, \big\|^2 \, \frac{dy}{\pi} = \|\psi\|^2, \;\; \psi \in \mathscr{H}.$$

The next lemma is a straightforward extension of [10, Corollary 3.1] where it is also shown that $R_{\mathbf{A}}(iy)$ maps $\mathcal{D}(H_{\mathrm{f}}^{\nu})$ into itself, for every $\nu > 0$.

Lemma 3.3. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1. Then, for all $\kappa, \nu \in \mathbb{R}$, we find $k_i \equiv k_i(\kappa, \nu, d_1, d_\rho) \in [1, \infty)$, $i = 1, 2$, such that, for all $y \in \mathbb{R}$, $\varepsilon \geqslant 0$, and $E \geqslant k_1$, there exist $\Upsilon_{\kappa,\nu}(iy), \widetilde{\Upsilon}_{\kappa,\nu}(iy) \in \mathscr{L}(\mathscr{H})$ satisfying*

$$R_{\mathbf{A}}(iy) \, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) = \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, R_{\mathbf{A}}(iy) \, \Upsilon_{\kappa,\nu}(iy) \tag{3.16}$$

$$= \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, \widetilde{\Upsilon}_{\kappa,\nu}(iy) \, R_{\mathbf{A}}(iy) , \tag{3.17}$$

on $\mathcal{D}(\check{H}_{\mathrm{f}}^{-\nu})$, and $\|\Upsilon_{\kappa,\nu}(iy)\|, \|\widetilde{\Upsilon}_{\kappa,\nu}(iy)\| \leqslant k_2$, where ρ is defined in Lemma 3.2.

Proof. Without loss of generality we may assume that $\varepsilon > 0$ for otherwise we could simply replace ν by $\nu + \kappa$ and f_0^{κ} by $f_0^0 = 1$. First, we assume in addition that $\nu \geqslant 0$. We observe that

$$T_0 := \big[\, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, , \, \boldsymbol{\alpha} \cdot \mathbf{A} \, \big] \, \check{H}_{\mathrm{f}}^{\nu} \, f_{\varepsilon}^{\kappa}(H_{\mathrm{f}}) = T_1 + T_2$$

on $\mathscr{D}$, where

$$T_1 := [\check{H}_{\mathrm{f}}^{-\nu} \, , \, \boldsymbol{\alpha} \cdot \mathbf{A}] \, \check{H}_{\mathrm{f}}^{\nu} , \qquad T_2 := \check{H}_{\mathrm{f}}^{-\nu} \, [f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, , \, \boldsymbol{\alpha} \cdot \mathbf{A}] \, f_{\varepsilon}^{\kappa}(H_{\mathrm{f}}) \, \check{H}_{\mathrm{f}}^{\nu} .$$

Due to (3.9) (or (3.11) with $\varepsilon = 0$) the operator T_1 extends to a bounded operator on $\mathscr{H}$ and $\|T_1\| \leqslant C_\nu / E^{1/2}$. According to (3.11) we further have $\|T_2\| \leqslant C_{\kappa,\nu}(d_1 + d_\rho)/E^{1/2}$. We pick some $\phi \in \mathscr{D}$ and compute

$$\big[\, R_{\mathbf{A}}(iy) \, , \, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, \big] \, (D_{\mathbf{A}} - iy) \, \phi = R_{\mathbf{A}}(iy) \, \big[\, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, , \, D_{\mathbf{A}} \, \big] \, \phi$$

$$= R_{\mathbf{A}}(iy) \, T_0 \, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, \phi$$

$$= R_{\mathbf{A}}(iy) \, \overline{T}_0 \, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, R_{\mathbf{A}}(iy) \, (D_{\mathbf{A}} - iy) \, \phi . \tag{3.18}$$

Since $(D_{\mathbf{A}} - iy) \, \mathscr{D}$ is dense in $\mathscr{H}$ and since $\check{H}_{\mathrm{f}}^{-\nu}$ and $f_{\varepsilon}^{\kappa}(H_{\mathrm{f}})$ are bounded (here we use that $\nu \geqslant 0$ and $\varepsilon > 0$), this identity implies

$$R_{\mathbf{A}}(iy) \, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) = \big(\mathbb{1} + R_{\mathbf{A}}(iy) \, \overline{T}_0 \big) \, \check{H}_{\mathrm{f}}^{-\nu} \, f_{\varepsilon}^{-\kappa}(H_{\mathrm{f}}) \, R_{\mathbf{A}}(iy) .$$

Taking the adjoint of the previous identity and replacing y by $-y$ we obtain

$$\check{H}_{\mathrm{f}}^{-\nu}\, f_\varepsilon^{-\kappa}(H_{\mathrm{f}})\, R_{\mathbf{A}}(iy) \,=\, R_{\mathbf{A}}(iy)\, \check{H}_{\mathrm{f}}^{-\nu}\, f_\varepsilon^{-\kappa}(H_{\mathrm{f}})\, (\mathbb{1} + T_0^*\, R_{\mathbf{A}}(iy))\,.$$

In view of the norm bounds on T_1 and T_2 we see that (3.16) and (3.17) are valid with $\Upsilon_{\kappa,\nu}(iy) := \sum_{\ell=0}^\infty \{-T_0^*\, R_{\mathbf{A}}(iy)\}^\ell$ and $\widetilde{\Upsilon}_{\kappa,\nu}(iy) := \sum_{\ell=0}^\infty \{-R_{\mathbf{A}}(iy)\, T_0^*\}^\ell$, provided that E is sufficiently large, depending only on κ, ν, d_1, and d_ρ, such that the Neumann series converge.
Now, let $\nu < 0$. Then we write T_0 on the domain $\mathscr{D}$ as

$$T_0 \,=\, \check{H}_{\mathrm{f}}^{-\nu}\, f_\varepsilon^{-\kappa}(H_{\mathrm{f}})\, \big[\boldsymbol{\alpha}\cdot\mathbf{A}\,,\, \check{H}_{\mathrm{f}}^{\nu}\, f_\varepsilon^{\kappa}(H_{\mathrm{f}})\big]\,,$$

and deduce that

$$R_{\mathbf{A}}(iy)\, \check{H}_{\mathrm{f}}^{\nu}\, f_\varepsilon^{\kappa}(H_{\mathrm{f}})\, (\mathbb{1} + \overline{T}_0\, R_{\mathbf{A}}(iy)) \,=\, \check{H}_{\mathrm{f}}^{\nu}\, f_\varepsilon^{\kappa}(H_{\mathrm{f}})\, R_{\mathbf{A}}(iy)$$

by a computation analogous to (3.18). Taking the adjoint of this identity with y replaced by $-y$ we get

$$\big(\mathbb{1} + R_{\mathbf{A}}(iy)\, T_0^*\big)\, \check{H}_{\mathrm{f}}^{\nu}\, f_\varepsilon^{\kappa}\, R_{\mathbf{A}}(iy) \,=\, R_{\mathbf{A}}(iy)\, \check{H}_{\mathrm{f}}^{\nu}\, f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,.$$

Next, we invert $\mathbb{1} + R_{\mathbf{A}}(iy)\, T_0^*$ by means of the same Neumann series as above. As a result we obtain

$$\check{H}_{\mathrm{f}}^{\nu} f_\varepsilon^{\kappa}(H_{\mathrm{f}})\, R_{\mathbf{A}}(iy) = R_{\mathbf{A}}(iy)\, \Upsilon_{\kappa,\nu}(iy)\, \check{H}_{\mathrm{f}}^{\nu} f_\varepsilon^{\kappa}(H_{\mathrm{f}}) = \widetilde{\Upsilon}_{\kappa,\nu}(iy)\, R_{\mathbf{A}}(iy)\, \check{H}_{\mathrm{f}}^{\nu} f_\varepsilon^{\kappa}(H_{\mathrm{f}}),$$

where the definition of $\Upsilon_{\kappa,\nu}$ and $\widetilde{\Upsilon}_{\kappa,\nu}$ has been extended to negative ν. It follows that $R_{\mathbf{A}}(iy)\, \Upsilon_{\kappa,\nu}(iy) = \widetilde{\Upsilon}_{\kappa,\nu}(iy)\, R_{\mathbf{A}}(iy)$ maps $\mathcal{D}(\check{H}_{\mathrm{f}}^{-\nu}) = \mathcal{D}(\check{H}_{\mathrm{f}}^{-\nu}\, f_\varepsilon^{-\kappa}(H_{\mathrm{f}})) = \mathrm{Ran}(\check{H}_{\mathrm{f}}^{\nu}\, f_\varepsilon^{\kappa}(H_{\mathrm{f}}))$ into itself and that (3.16) and (3.17) still hold true when ν is negative. □

In order to control the Coulomb singularity $1/|\mathbf{x}|$ in terms of $|D_{\mathbf{A}}|$ and H_{f} in the proof of the following corollary, we shall employ the bound [10, Theorem 2.3]

$$\frac{2}{\pi}\frac{1}{|\mathbf{x}|} \,\leqslant\, |D_{\mathbf{A}}| + H_{\mathrm{f}} + k\, d_1^2\,, \tag{3.19}$$

which holds true in sense of quadratic forms on $\mathcal{Q}(|D_{\mathbf{A}}|) \cap \mathcal{Q}(H_{\mathrm{f}})$. Here $k \in (0,\infty)$ is some universal constant. We abbreviate the sign function of the Dirac operator, which can be represented as a strongly convergent principal value [6, Lemma VI.5.6], by

$$S_{\mathbf{A}}\, \psi \,:=\, D_{\mathbf{A}}\, |D_{\mathbf{A}}|^{-1}\, \psi \,=\, \lim_{\tau\to\infty} \int_{-\tau}^{\tau} R_{\mathbf{A}}(iy)\, \psi\, \frac{dy}{\pi}\,. \tag{3.20}$$

We recall from [10, Lemma 3.3] that $S_{\mathbf{A}}$ maps $\mathcal{D}(H_{\mathrm{f}}^{\nu})$ into itself, for every $\nu > 0$. This can also be read off from the proof of the next corollary.

COROLLARY 3.4. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1. Let $\kappa, \nu \in \mathbb{R}$. Then we find some $C \equiv C(\kappa, \nu, d_1, d_\rho) \in (0,\infty)$ such that, for all $\gamma, \delta, \sigma, \tau \geqslant 0$*

with $\gamma+\delta+\sigma+\tau\leqslant 1/2$ *and all* $\varepsilon\geqslant 0$, $E\geqslant k_1$,

$$\big\|\,\check{H}_{\mathrm{f}}^{\nu}\,f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,S_{\mathbf{A}}\,\check{H}_{\mathrm{f}}^{-\nu}\,f_\varepsilon^{-\kappa}(H_{\mathrm{f}})\,\big\|\leqslant C, \tag{3.21}$$

$$\big\|\,|D_{\mathbf{A}}|^{1/2}\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\,f_\varepsilon^{\sigma}(H_{\mathrm{f}})\,[S_{\mathbf{A}}\,,\,f_\varepsilon^{\kappa}(H_{\mathrm{f}})]\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\,f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\big\|\leqslant C, \tag{3.22}$$

$$\big\|\,|\mathbf{x}|^{-1/2}\,\check{H}_{\mathrm{f}}^{\nu}\,f_\varepsilon^{\sigma}(H_{\mathrm{f}})\,[S_{\mathbf{A}}\,,\,f_\varepsilon^{\kappa}(H_{\mathrm{f}})]\,\check{H}_{\mathrm{f}}^{-\nu-\sigma-\tau}\,f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\big\|\leqslant C. \tag{3.23}$$

(k_1 is the constant appearing in Lemma 3.3, $\check{H}_{\mathrm{f}}$ is given by (3.8)*, f_ε by* (3.10)*.)*

Proof. First, we prove (3.22). Using (3.20), writing

$$[R_{\mathbf{A}}(iy)\,,\,f_\varepsilon^{\kappa}(H_{\mathrm{f}})]\;=\;R_{\mathbf{A}}(iy)\,[f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,,\,\boldsymbol{\alpha}\cdot\mathbf{A}]\,R_{\mathbf{A}}(iy)$$

on $\mathscr{D}$ and employing (3.16), (3.17), and (3.11) we obtain the following estimate, for all $\varphi,\psi\in\mathscr{D}$, and $E\geqslant k_1$,

$$\begin{aligned}
&\big|\big\langle\,|D_{\mathbf{A}}|^{1/2}\,\varphi\,\big|\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\,f_\varepsilon^{\sigma}(H_{\mathrm{f}})\,[S_{\mathbf{A}}\,,\,f_\varepsilon^{\kappa}(H_{\mathrm{f}})]\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\,f_\varepsilon(H_{\mathrm{f}})^{-\kappa+\tau}\,\psi\,\big\rangle\big|\\
&\leqslant\int_{\mathbb{R}}\Big|\Big\langle\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\,|D_{\mathbf{A}}|^{1/2}\,\varphi\,\Big|\,f_\varepsilon^{\sigma}(H_{\mathrm{f}})\,[f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,,\,R_{\mathbf{A}}(iy)]\,\times\\
&\qquad\times\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\,f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\psi\,\Big\rangle\Big|\,\frac{dy}{\pi}\\
&=\int_{\mathbb{R}}\Big|\Big\langle\,\varphi\,\Big|\,|D_{\mathbf{A}}|^{1/2}\,R_{\mathbf{A}}(iy)\,\Upsilon_{\sigma,\nu+\gamma}(iy)\,\check{H}_{\mathrm{f}}^{\nu+\gamma}\,f_\varepsilon^{\sigma}(H_{\mathrm{f}})\,[f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,,\,\boldsymbol{\alpha}\cdot\mathbf{A}]\,\times\\
&\qquad\times\,\check{H}_{\mathrm{f}}^{-\nu+\delta}\,f_\varepsilon^{-\kappa+\tau}(H_{\mathrm{f}})\,\widetilde{\Upsilon}_{\kappa-\tau,\nu-\delta}(iy)\,R_{\mathbf{A}}(iy)\,\psi\,\Big\rangle\Big|\,\frac{dy}{\pi}\\
&\leqslant C_{\kappa,\nu}\,(d_1+d_\rho)\,E^{\gamma+\delta+\sigma+\tau-1/2}\,\sup_{y\in\mathbb{R}}\{\|\Upsilon_{\sigma,\nu+\gamma}(iy)\|\,\|\widetilde{\Upsilon}_{\kappa-\tau,\nu-\delta}(iy)\|\}\\
&\qquad\cdot\Big(\int_{\mathbb{R}}\big\|\,|D_{\mathbf{A}}|^{1/2}\,R_{\mathbf{A}}(iy)\,\varphi\,\big\|^2\,\frac{dy}{\pi}\Big)^{1/2}\Big(\int_{\mathbb{R}}\big\|\,R_{\mathbf{A}}(iy)\,\psi\,\big\|^2\,\frac{dy}{\pi}\Big)^{1/2}\\
&\leqslant C_{\kappa,\nu,d_1,d_\rho}\,E^{\gamma+\delta+\sigma+\tau-1/2}\,\|\varphi\|\,\|\psi\|\,.
\end{aligned}$$

This estimate shows that the vector in the right entry of the scalar product in the first line belongs to $\mathcal{D}((|D_{\mathbf{A}}|^{1/2})^*)=\mathcal{D}(|D_{\mathbf{A}}|^{1/2})$ and that (3.22) holds true. Next, we observe that (3.23) follows from (3.22) and (3.19). Finally, (3.21) follows from $\|X\|\leqslant\mathrm{const}(\nu,\kappa,d_1,d_\rho)$, where $X:=\check{H}_{\mathrm{f}}^{\nu}\,f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,[S_{\mathbf{A}}\,,\,\check{H}_{\mathrm{f}}^{-\nu}\,f_\varepsilon^{-\kappa}(H_{\mathrm{f}})]$. Such a bound on $\|X\|$ is, however, an immediate consequence of (3.22) (where we can choose $\varepsilon=0$) because

$$X\;=\;[\check{H}_{\mathrm{f}}^{\nu}\,,\,S_{\mathbf{A}}]\,\check{H}_{\mathrm{f}}^{-\nu}\;+\;\check{H}_{\mathrm{f}}^{\nu}\,[f_\varepsilon^{\kappa}(H_{\mathrm{f}})\,,\,S_{\mathbf{A}}]\,f_\varepsilon^{-\kappa}(H_{\mathrm{f}})\,\check{H}_{\mathrm{f}}^{-\nu}$$

on the domain $\mathscr{D}$. □

4. Non-relativistic QED

The Pauli-Fierz operator for a molecular system with static nuclei and $N\in\mathbb{N}$ electrons interacting with the quantized radiation field is acting in the Hilbert space

$$\mathscr{H}_N\;:=\;\mathcal{A}_N L^2\big((\mathbb{R}^3\times\mathbb{Z}_4)^N\big)\otimes\mathscr{F}_{\mathrm{b}}\,, \tag{4.1}$$

where $\mathcal{A}_N = \mathcal{A}_N^2 = \mathcal{A}_N^*$ denotes anti-symmetrization,

$$(\mathcal{A}_N \, \Psi)(X) := \frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} (-1)^\pi \, \Psi\big(\mathbf{x}_{\pi(1)}, \varsigma_{\pi(1)}, \ldots, \mathbf{x}_{\pi(N)}, \varsigma_{\pi(N)}\big),$$

for $\Psi \in L^2((\mathbb{R}^3 \times \mathbb{Z}_4)^N)$ and a.e. $X = (\mathbf{x}_i, \varsigma_i)_{i=1}^N \in (\mathbb{R}^3 \times \mathbb{Z}_4)^N$. a priori it is defined on the dense domain

$$\mathscr{D}_N := \mathcal{A}_N C_0^\infty\big((\mathbb{R}^3 \times \mathbb{Z}_4)^N\big) \otimes \mathscr{C}_0 ,$$

the tensor product understood in the algebraic sense, by

$$H_{\mathrm{nr}}^V \equiv H_{\mathrm{nr}}^V(\mathbf{G}) := \sum_{i=1}^N (D_{\mathbf{A}}^{(i)})^2 + V + H_{\mathrm{f}} . \tag{4.2}$$

A superscript (i) indicates that the operator below is acting on the pair of variables $(\mathbf{x}_i, \varsigma_i)$. In fact, the operator defined in (4.2) is a two-fold copy of the usual Pauli-Fierz operator which acts on two-spinors and the energy has been shifted by N in (4.2). For (3.5) implies

$$D_{\mathbf{A}}^2 = \mathcal{T}_{\mathbf{A}} \oplus \mathcal{T}_{\mathbf{A}} , \quad \mathcal{T}_{\mathbf{A}} := \big(\boldsymbol{\sigma} \cdot (-i\nabla_{\mathbf{x}} + \mathbf{A})\big)^2 + 1 . \tag{4.3}$$

Here $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector containing the Pauli matrices (when α_j, $j \in \{0,1,2,3\}$, are given in Dirac's standard representation). We write H_{nr}^V in the form (4.2) to maintain a unified notation throughout this paper.
We shall only make use of the following properties of the potential V.

HYPOTHESIS 4.1. *V can be written as $V = V_+ - V_-$, where $V_\pm \geqslant 0$ is a symmetric operator acting in $\mathcal{A}_N L^2\big((\mathbb{R}^3 \times \mathbb{Z}_4)^4\big)$ such that $\mathscr{D}_N \subset \mathcal{D}(V_\pm)$. There exist $a \in (0,1)$ and $b \in (0,\infty)$ such that $V_- \leqslant a\, H_{\mathrm{nr}}^0 + b$ in the sense of quadratic forms on $\mathscr{D}_N$.*

Example. The Coulomb potential generated by $K \in \mathbb{N}$ fixed nuclei located at the positions $\{\mathbf{R}_1, \ldots, \mathbf{R}_K\} \subset \mathbb{R}^3$ is given as

$$V_{\mathrm{C}}(X) := -\sum_{i=1}^N \sum_{k=1}^K \frac{e^2 \, Z_k}{|\mathbf{x}_i - \mathbf{R}_k|} + \sum_{\substack{i,j=1 \\ i<j}}^N \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} , \tag{4.4}$$

for some $e, Z_1, \ldots, Z_K > 0$ and a.e. $X = (\mathbf{x}_i, \varsigma_i)_{i=1}^N \in (\mathbb{R}^3 \times \mathbb{Z}_4)^N$. It is well-known that V_{C} is infinitesimally H_{nr}^0-bounded and that V_{C} fulfills Hypothesis 4.1. ⋄

It follows immediately from Hypothesis 4.1 that H_{nr}^V has a self-adjoint Friedrichs extension – henceforth denoted by the same symbol H_{nr}^V – and that $\mathscr{D}_N$ is a form core for H_{nr}^V. Moreover, we have

$$(D_{\mathbf{A}}^{(1)})^2, \ldots, (D_{\mathbf{A}}^{(N)})^2, V_+, H_{\mathrm{f}} \leqslant H_{\mathrm{nr}}^{V_+} \leqslant (1-a)^{-1} \, (H_{\mathrm{nr}}^V + b) \tag{4.5}$$

on $\mathscr{D}_N$. In [4] it is shown that $\mathcal{D}((H_{\mathrm{nr}}^V)^{n/2}) \subset \mathcal{D}(H_{\mathrm{f}}^{n/2})$, for every $n \in \mathbb{N}$. We re-derive this result by means of Corollary 2.3 in the next theorem where

$$E_{\mathrm{nr}} := \inf \sigma[H_{\mathrm{nr}}^V] , \qquad H_{\mathrm{nr}}' := H_{\mathrm{nr}}^V - E_{\mathrm{nr}} + 1 .$$

Theorem 4.2. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1 and that V fulfills Hypothesis 4.1. Assume in addition that*

$$2\int \omega(k)^{\ell}\,\|\nabla_{\mathbf{x}}\wedge\mathbf{G}(k)\|_{\infty}^{2}\,dk \,\leqslant\, d_{\ell+2}^{2}\,, \tag{4.6}$$

$$\int \omega(k)^{\ell}\,\|\nabla_{\mathbf{x}}\cdot\mathbf{G}(k)\|_{\infty}^{2}\,dk \,\leqslant\, d_{\ell+2}^{2}\,, \tag{4.7}$$

for all $\ell\in\{-1,0,1,2,\ldots\}$. Then, for every $n\in\mathbb{N}$, we have $\mathcal{D}((H_{\mathrm{nr}}^{V})^{n/2})\subset\mathcal{D}(H_{\mathrm{f}}^{n/2})$, $H_{\mathrm{f}}^{n/2}\,(H'_{\mathrm{nr}})^{-n/2}$ maps $\mathcal{D}(H_{\mathrm{nr}}^{V})$ into itself, and

$$\big\|\,H_{\mathrm{f}}^{n/2}\,(H'_{\mathrm{nr}})^{-n/2}\,\big\|\,\leqslant\,C(N,n,a,b,d_{-1},d_1,d_{5+n})\,(|E_{\mathrm{nr}}|+1)^{(3n-2)/2}\,,$$
$$\big\|\,[H_{\mathrm{f}}^{n/2}\,,\,H_{\mathrm{nr}}^{V}]\,(H'_{\mathrm{nr}})^{-n/2}\,\big\|\,\leqslant\,C'(N,n,a,b,d_{-1},d_1,d_{5+n})\,(|E_{\mathrm{nr}}|+1)^{(3n-1)/2}\,.$$

Proof. We pick the function f_ε defined in (3.10) with $E=1$ and verify that the operators $F_\varepsilon^n := f_\varepsilon^{n/2}(H_{\mathrm{f}})$, $\varepsilon>0$, $n\in\mathbb{N}$, and H'_{nr} fulfill the conditions (a), (b), and (c') of Theorem 2.1 and Corollary 2.2 with $m=\infty$. Then the assertion follows from Corollary 2.3. We set $\check{H}_{\mathrm{f}}:=H_{\mathrm{f}}+E$ in what follows. By means of (4.5) we find

$$\langle\,\Psi\,|\,F_\varepsilon^2\,\Psi\,\rangle\leqslant\langle\,\Psi\,|\,\check{H}_{\mathrm{f}}\,\Psi\,\rangle\leqslant\frac{E_{\mathrm{nr}}+b+E}{1-a}\,\langle\,\Psi\,|\,H'_{\mathrm{nr}}\,\Psi\,\rangle\,, \tag{4.8}$$

for all $\Psi\in\mathscr{D}_N$, which is Condition (b). Next, we observe that F_ε maps $\mathscr{D}_N$ into itself. Employing (4.5) once more and using $-V_-\leqslant 0$ and the fact that $V_+\geqslant 0$ and F_ε act on different tensor factors we deduce that

$$\begin{aligned}\big\langle\,F_\varepsilon\,\Psi\,\big|\,(V+H_{\mathrm{f}})\,F_\varepsilon\,\Psi\,\big\rangle\,&\leqslant\,\|f_\varepsilon\|_\infty\,\big\langle\,\Psi\,\big|\,(V_++H_{\mathrm{f}})\,\Psi\,\big\rangle\\&\leqslant\,\|f_\varepsilon\|_\infty\,\frac{E_{\mathrm{nr}}+b+E}{1-a}\,\langle\,\Psi\,|\,H'_{\mathrm{nr}}\,\Psi\,\rangle\,,\end{aligned} \tag{4.9}$$

for every $\Psi\in\mathscr{D}_N$. Thanks to (3.11) with $\kappa=1/2$, $\nu=\gamma=\delta=\sigma=\tau=0$, and (4.5) we further find some $C\in(0,\infty)$ such that

$$\begin{aligned}\big\|\,D_{\mathbf{A}}^{(i)}\,F_\varepsilon\,\Psi\,\big\|^2&\leqslant 2\,\|f_\varepsilon\|_\infty\,\|D_{\mathbf{A}}^{(i)}\,\Psi\|^2+2\,\|f_\varepsilon\|_\infty\,\big\|\,F_\varepsilon^{-1}\,[\boldsymbol{\alpha}\cdot\mathbf{A}\,,\,F_\varepsilon]\,\big\|^2\,\|\Psi\|^2\\&\leqslant C\,\|f_\varepsilon\|_\infty\,\langle\,\Psi\,|\,H'_{\mathrm{nr}}\,\Psi\,\rangle\,,\end{aligned} \tag{4.10}$$

for all $\Psi\in\mathscr{D}_N$. (4.9) and (4.10) together show that Condition (a) is fulfilled, too. Finally, we verify the bound in (c'). We use

$$[\boldsymbol{\alpha}\cdot(-i\nabla_{\mathbf{x}})\,,\,\boldsymbol{\alpha}\cdot\mathbf{A}]\,=\,\boldsymbol{\Sigma}\cdot\mathbf{B}-i\,(\nabla_{\mathbf{x}}\cdot\mathbf{A})\,,$$

where $\mathbf{B}:=a^\dagger(\nabla_{\mathbf{x}}\wedge\mathbf{G})+a(\nabla_{\mathbf{x}}\wedge\mathbf{G})$ is the magnetic field and the j-th entry of the formal vector $\boldsymbol{\Sigma}$ is $-i\,\epsilon_{jk\ell}\,\alpha_k\,\alpha_\ell$, $j,k,\ell\in\{1,2,3\}$, to write the square of the Dirac operator on the domain $\mathscr{D}$ as

$$D_{\mathbf{A}}^2\,=\,D_{\mathbf{0}}^2+\boldsymbol{\Sigma}\cdot\mathbf{B}-i\,(\nabla_{\mathbf{x}}\cdot\mathbf{A})+(\boldsymbol{\alpha}\cdot\mathbf{A})^2+2\,\boldsymbol{\alpha}\cdot\mathbf{A}\,\boldsymbol{\alpha}\cdot(-i\nabla_{\mathbf{x}})\,.$$

This yields

$$[H'_{\rm nr}, F_\varepsilon^n] = \sum_{i=1}^N \big[(D_{\mathbf{A}}^{(i)})^2, F_\varepsilon^n\big] = \sum_{i=1}^N \big\{ [\mathbf{\Sigma}\cdot\mathbf{B}^{(i)}\,,\,F_\varepsilon^n] - i\,[(\nabla_{\mathbf{x}}\cdot\mathbf{A}^{(i)})\,,\,F_\varepsilon^n]$$
$$+\,\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,[\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,,\,F_\varepsilon^n] + [\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,,\,F_\varepsilon^n]\,(2D_{\mathbf{A}}^{(i)} - \boldsymbol{\alpha}\cdot\mathbf{A}^{(i)} - 2\beta)\,\big\}$$

on $\mathscr{D}_N$. For every $i\in\{1,\dots,N\}$, we further write

$$[\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,,\,F_\varepsilon^n]\,D_{\mathbf{A}}^{(i)} \;=\; Q_{\varepsilon,n}^{(i)}\,\big(\,D_{\mathbf{A}}^{(i)}\,F_\varepsilon^{n-1} - Q_{\varepsilon,n-1}^{(i)}\,F_\varepsilon^{n-2}\,\big)$$

on $\mathscr{D}_N$, where

$$Q_{\varepsilon,n}^{(i)} \;:=\; [\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,,\,F_\varepsilon^n]\,F_\varepsilon^{1-n}\,,\quad n\in\mathbb{N}\,,\qquad Q_{\varepsilon,0}^{(i)} \;:=\; 0\,. \tag{4.11}$$

According to (3.11) we have $\|Q_{\varepsilon,n}^{(i)}\| \leqslant n\,2^{(n+2)/2}\,(d_1 + d_{3+n})$, $\|\check{H}_{\rm f}^{1/2}\,Q_{\varepsilon,n}^{(i)}\,\check{H}_{\rm f}^{-1/2}\| \leqslant n\,2^{(n+3)/2}(d_1+d_{4+n})$. Likewise, we write

$$[\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,,\,F_\varepsilon^n]\,\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)} \;=\; Q_{\varepsilon,n}^{(i)}\,\big(\,\{\boldsymbol{\alpha}\cdot\mathbf{A}^{(i)}\,\check{H}_{\rm f}^{-1/2}\}\,\check{H}_{\rm f}^{1/2}\,F_\varepsilon^{n-1} - Q_{\varepsilon,n-1}^{(i)}\,F_\varepsilon^{n-2}\,\big)$$

on $\mathscr{D}_N$, where $\|\boldsymbol{\alpha}\cdot\mathbf{A}\,\check{H}_{\rm f}^{-1/2}\|^2 \leqslant 2\,d_0^2 + 4\,d_{-1}^2$ by (3.7). Furthermore, we observe that Lemma 3.2 is applicable to $\mathbf{\Sigma}\cdot\mathbf{B}$ as well instead of $\boldsymbol{\alpha}\cdot\mathbf{A}$; we simply have to replace the form factor $\mathbf{G}$ by $\nabla_{\mathbf{x}}\wedge\mathbf{G}$ and to notice that $\|\mathbf{\Sigma}\cdot\mathbf{v}\|_{\mathscr{L}(\mathbb{C}^4)} = |\mathbf{v}|$, $\mathbf{v}\in\mathbb{R}^3$, in analogy to (3.6). Note that the indices of d_ℓ are shifted by 2 because of (4.6). Finally, we observe that Lemma 3.2 is applicable to $\nabla_{\mathbf{x}}\cdot\mathbf{A}$, too. To this end we have to replace $\mathbf{G}$ by $(\nabla_{\mathbf{x}}\cdot\mathbf{G},0,0)$ and d_ℓ by some universal constant times $d_{2+\ell}$ because of (4.7). Taking all these remarks into account we arrive at

$$\big|\big\langle\,\Psi_1\,\big|\,[H'_{\rm nr}\,,\,F_\varepsilon^n]\,\Psi_2\,\big\rangle\big| \;\leqslant\; \sum_{i=1}^N \Big\{\,\|\Psi_1\|\,\big\|\,[\mathbf{\Sigma}\cdot\mathbf{B}^{(i)}\,,\,F_\varepsilon^n]\,F_\varepsilon^{1-n}\,\big\|\,\|F_\varepsilon^{n-1}\,\Psi_2\|$$
$$+\,\|\Psi_1\|\,\big\|\,[\mathrm{div}\,\mathbf{A}^{(i)}\,,\,F_\varepsilon^n]\,F_\varepsilon^{1-n}\,\big\|\,\|F_\varepsilon^{n-1}\,\Psi_2\|$$
$$+\,\|\Psi_1\|\,\|\boldsymbol{\alpha}\cdot\mathbf{A}\,\check{H}_{\rm f}^{-1/2}\|\,\big\|\,\check{H}_{\rm f}^{1/2}\,Q_{\varepsilon,n}^{(i)}\,\check{H}_{\rm f}^{-1/2}\,\big\|\,\|\check{H}_{\rm f}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|$$
$$+\,\|\Psi_1\|\,\|Q_{\varepsilon,n}^{(i)}\|\,\big(\,2\,\|D_{\mathbf{A}}^{(i)}\,F_\varepsilon^{n-1}\,\Psi_2\| + \|\boldsymbol{\alpha}\cdot\mathbf{A}\,\check{H}_{\rm f}^{-1/2}\|\,\|\check{H}_{\rm f}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|\,\big)$$
$$+\,3\,\|\Psi_1\|\,\|Q_{\varepsilon,n}^{(i)}\|\,\|Q_{\varepsilon,n-1}^{(i)}\|\,\|F_\varepsilon^{n-2}\,\Psi_2\| + 2\,\|\Psi_1\|\,\|Q_{\varepsilon,n}^{(i)}\|\,\|\beta\|\,\|F_\varepsilon^{n-1}\,\Psi_2\|\,\Big\}\,,$$

for all $\Psi_1,\Psi_2\in\mathscr{D}_N$. From this estimate, Lemma 3.2, and (4.5) we readily infer that Condition (c') is valid with $c_n = (|E_{\rm nr}|+1)\,C''(N,n,a,b,d_{-1},\dots,d_{5+n})$. □

5. The semi-relativistic Pauli-Fierz operator

The semi-relativistic Pauli-Fierz operator is also acting in the Hilbert space $\mathscr{H}_N$ introduced in (4.1). It is obtained by substituting the non-local operator $|D_{\mathbf{A}}|$ for $D_{\mathbf{A}}^2$ in $H_{\rm nr}^V$. We thus define, a priori on the dense domain $\mathscr{D}_N$,

$$H_{\rm sr}^V \;\equiv\; H_{\rm sr}^V(\mathbf{G}) \;:=\; \sum_{i=1}^N |D_{\mathbf{A}}^{(i)}| \,+\, V \,+\, H_{\rm f}\,,$$

where V is assumed to fulfill Hypothesis 4.1 with H^0_{nr} replaced by H^0_{sr}. To ensure that in the case of the Coulomb potential V_{C} defined in (4.4) this yields a well-defined self-adjoint operator we have to impose appropriate restrictions on the nuclear charges.

Example. In Proposition A.1 we show that $H^{V_{\mathrm{C}}}_{\mathrm{sr}}$ is semi-bounded below on $\mathscr{D}_N$ provided that $Z_k \in (0, 2/\pi e^2]$, for all $k \in \{1, \dots, K\}$. Its proof is actually a straightforward consequence of (3.19) and a commutator estimate obtained in [10]. If all atomic numbers Z_k are strictly less than $2/\pi e^2$ we thus find $a \in (0,1)$ and $b \in (0,\infty)$ such that

$$\sum_{i=1}^{N}\sum_{k=1}^{K} \frac{e^2\, Z_k}{|\mathbf{x}_i - \mathbf{R}_k|} \;\leqslant\; a\, H^0_{\mathrm{sr}} + b \tag{5.1}$$

in the sense of quadratic forms on $\mathscr{D}_N$. In particular, V_{C} fulfills Hypothesis 4.1 with H^0_{nr} replaced by H^0_{sr} as long as $Z_k \in (0, 2/\pi e^2)$, for $k \in \{1, \dots, K\}$. $\diamond$

For potentials V as above H^V_{sr} has a self-adjoint Friedrichs extension which we denote again by the same symbol H^V_{sr}. Moreover, $\mathscr{D}_N$ is a form core for H^V_{sr} and we have the following analogue of (4.5),

$$|D^{(1)}_{\mathbf{A}}|, \dots, |D^{(N)}_{\mathbf{A}}|,\, V_+,\, H_{\mathrm{f}} \;\leqslant\; H^{V_+}_{\mathrm{sr}} \;\leqslant\; (1-a)^{-1}\,(H^V_{\mathrm{sr}} + b) \tag{5.2}$$

on $\mathscr{D}_N$. In order to apply Corollary 2.3 to the semi-relativistic Pauli-Fierz operator we recall the following special case of [7, Corollary 3.7]:

Lemma 5.1. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1. Let $\tau \in (0,1]$. Then there exist $\delta > 0$ and $C \equiv C(\delta, \tau, d_1) \in (0,\infty)$ such that*

$$C + |D_{\mathbf{A}}| + \tau\, H_{\mathrm{f}} \geqslant \delta\,(|D_{\mathbf{0}}| + H_{\mathrm{f}}) \geqslant \delta\,(|D_{\mathbf{0}}| + \tau\, H_{\mathrm{f}}) \;\geqslant\; \delta^2\,|D_{\mathbf{A}}| - \delta\, C \tag{5.3}$$

in the sense of quadratic forms on $\mathscr{D}$.

In the next theorem we re-derive the higher order estimates obtained in [4] for the semi-relativistic Pauli-Fierz operator by means of Corollary 2.3. (The second estimate of Theorem 5.2 is actually slightly stronger than the corresponding one stated in [4].) The estimates of the following proof are also employed in Section 6 where we treat the no-pair operator. We set

$$E_{\mathrm{sr}} \;:=\; \inf \sigma[H_{\mathrm{sr}}]\,, \qquad H'_{\mathrm{sr}} \;:=\; H^V_{\mathrm{sr}} - E_{\mathrm{sr}} + 1\,.$$

Theorem 5.2. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1 and that V fulfills Hypothesis 4.1 with H^0_{nr} replaced by H^0_{sr}. Then, for every $m \in \mathbb{N}$, it follows that $\mathcal{D}((H^V_{\mathrm{sr}})^{m/2}) \subset \mathcal{D}(H_{\mathrm{f}}^{m/2})$, $H_{\mathrm{f}}^{m/2}\,(H'_{\mathrm{sr}})^{-m/2}$ maps $\mathcal{D}(H^V_{\mathrm{sr}})$ into itself, and*

$$\big\|\, H_{\mathrm{f}}^{m/2}\,(H'_{\mathrm{sr}})^{-m/2}\,\big\| \;\leqslant\; C(N,m,a,b,d_1,d_{3+m})\,(|E_{\mathrm{sr}}|+1)^{(3m-2)/2}\,,$$

$$\big\|\,[H_{\mathrm{f}}^{m/2}\,,\,H^V_{\mathrm{sr}}]\,(H'_{\mathrm{sr}})^{-m/2}\,\big\| \;\leqslant\; C'(N,m,a,b,d_1,d_{3+m})\,(|E_{\mathrm{sr}}|+1)^{(3m-1)/2}\,.$$

Proof. Let $m \in \mathbb{N}$. We pick the function f_ε defined in (3.10) with $E = k_1 \vee C$. (k_1 is the constant appearing in Lemma 3.3 with $\kappa = m/2$, $\nu = 0$, and depends on m, d_1, and d_{3+m}; C is the one in (5.3).) We fix some $n \in \mathbb{N}$, $n \leqslant m$, and verify Conditions (a), (b), and (c') of Theorem 2.1 and Corollary 2.2 with $F_\varepsilon = f_\varepsilon^{1/2}(H_{\mathrm{f}})$, $\varepsilon > 0$. The estimates (4.8) and (4.9) are still valid without any further change when the subscript nr is replaced by sr. Employing (5.3) twice and using (5.2) we obtain the following substitute of (4.10),

$$\begin{aligned}\big\langle F_\varepsilon \Psi \,\big|\, |D_{\mathbf{A}}| F_\varepsilon \Psi \big\rangle &\leqslant \delta^{-1} \| |D_{\mathbf{0}}|^{1/2} F_\varepsilon \Psi\|^2 + \delta^{-1} \|\check{H}_{\mathrm{f}}^{1/2} F_\varepsilon \Psi\|^2 \\ &\leqslant \delta^{-1} \|f_\varepsilon\|_\infty \big(\| |D_{\mathbf{0}}|^{1/2} \Psi\|^2 + \|\check{H}_{\mathrm{f}}^{1/2} \Psi\|^2\big) \leqslant C' \|f_\varepsilon\|_\infty \big\langle \Psi \,\big|\, H'_{\mathrm{sr}} \Psi \big\rangle ,\end{aligned}$$

for all $\Psi \in \mathscr{D}_N$. Altogether we see that Conditions (a) and (b) are satisfied. In order to verify (c') we set

$$U^{(i)}_{\varepsilon,n} := [S^{(i)}_{\mathbf{A}}, F^n_\varepsilon]\, F_\varepsilon^{1-n} = F^n_\varepsilon\, [F_\varepsilon^{-n}, S^{(i)}_{\mathbf{A}}]\, F_\varepsilon , \qquad i \in \{1, \ldots, N\} . \tag{5.4}$$

By virtue of (3.22) we know that the norms of $U^{(i)}_{\varepsilon,n}$ and $U^{(i)}_{\varepsilon,n} |D^{(i)}_{\mathbf{A}}|^{1/2}$ are bounded uniformly in $\varepsilon > 0$ by some constant, $C \in (0, \infty)$, that depends only on n, d_1, and d_{3+n}. We employ the notation (4.11) and (5.4) to write

$$\begin{aligned}[H'_{\mathrm{sr}}, F^n_\varepsilon] &= \sum_{i=1}^N \big[\, |D^{(i)}_{\mathbf{A}}|, F^n_\varepsilon \,\big] = \sum_{i=1}^N \big[\, S^{(i)}_{\mathbf{A}} D^{(i)}_{\mathbf{A}}, F^n_\varepsilon \,\big] \\ &= \sum_{i=1}^N \Big\{ \{U^{(i)}_{\varepsilon,n} |D^{(i)}_{\mathbf{A}}|^{1/2}\}\, S^{(i)}_{\mathbf{A}}\, |D^{(i)}_{\mathbf{A}}|^{1/2} F^{n-1}_\varepsilon \\ &\qquad\qquad - U^{(i)}_{\varepsilon,n} Q^{(i)}_{\varepsilon,n-1} F^{n-2}_\varepsilon + S^{(i)}_{\mathbf{A}} Q^{(i)}_{\varepsilon,n} F^{n-1}_\varepsilon \Big\}.\end{aligned}$$

The previous identity, (5.2), and $|D_{\mathbf{A}}| \geqslant 1$ permit to get

$$\begin{aligned}\big|\big\langle \Psi_1 \,\big|\, [H'_{\mathrm{sr}}, F^n_\varepsilon]\, \Psi_2 \big\rangle\big| &\leqslant \sum_{i=1}^N \|\Psi_1\| \big\{ C \,\big\| |D^{(i)}_{\mathbf{A}}|^{1/2} F^{n-1}_\varepsilon \Psi_2 \big\| \\ &\qquad + C \|Q^{(i)}_{\varepsilon,n}\| \|F^{n-2}_\varepsilon \Psi_2\| + \|Q^{(i)}_{\varepsilon,n}\| \|F^{n-1}_\varepsilon \Psi_2\| \big\} \\ &\leqslant c_n \big\{ \|\Psi_1\|^2 + \big\langle F^{n-1}_\varepsilon \Psi_2 \,\big|\, H'_{\mathrm{sr}} F^{n-1}_\varepsilon \Psi_2 \big\rangle \big\} ,\end{aligned}$$

for all $\Psi_1, \Psi_2 \in \mathscr{D}_N$ and some constant $c_n = C''(n, a, b, d_1, d_{3+n})\, (|E_{\mathrm{sr}}| + 1)$. So (c') is fulfilled also and the assertion follows from Corollary 2.3. □

6. The no-pair operator

We introduce the spectral projections

$$P^+_{\mathbf{A}} := E_{[0,\infty)}(D_{\mathbf{A}}) = \frac{1}{2} \mathbb{1} + \frac{1}{2} S_{\mathbf{A}} , \qquad P^-_{\mathbf{A}} := \mathbb{1} - P^+_{\mathbf{A}} . \tag{6.1}$$

The no-pair operator acts in the projected Hilbert space

$$\mathscr{H}^+_N \equiv \mathscr{H}^+_N(\mathbf{G}) := P^+_{\mathbf{A},N} \mathscr{H}_N , \qquad P^+_{\mathbf{A},N} := \prod_{i=1}^N P^{+,(i)}_{\mathbf{A}} ,$$

and is a priori defined on the dense domain $P^+_{\mathbf{A},N}\,\mathscr{D}_N$ by

$$H^V_{\mathrm{np}} \equiv H^V_{\mathrm{np}}(\mathbf{G}) := P^+_{\mathbf{A},N}\Big\{\sum_{i=1}^N D^{(i)}_{\mathbf{A}} + V + H_{\mathrm{f}}\Big\}P^+_{\mathbf{A},N}\,.$$

Notice that all operators $D^{(1)}_{\mathbf{A}},\dots,D^{(N)}_{\mathbf{A}}$ and $P^{+,(1)}_{\mathbf{A}},\dots,P^{+,(N)}_{\mathbf{A}}$ commute in pairs owing to the fact that the components of the vector potential $A^{(i)}(\mathbf{x})$, $A^{(j)}(\mathbf{y})$, $\mathbf{x},\mathbf{y}\in\mathbb{R}^3$, $i,j\in\{1,2,3\}$, commute in the sense that all their spectral projections commute; see the appendix to [9] for more details. (Here we use the assumption that $\mathbf{G}_{\mathbf{x}}(-\mathbf{k},\lambda)=\overline{\mathbf{G}_{\mathbf{x}}(\mathbf{k},\lambda)}$.) So the order of the application of the projections $P^{+,(i)}_{\mathbf{A}}$ is immaterial. In this section we restrict the discussion to the case where V is given by the Coulomb potential V_{C} defined in (4.4). To have a handy notation we set

$$v_i := -\sum_{k=1}^K \frac{e^2\,Z_k}{|\mathbf{x}_i-\mathbf{R}_k|}\,,\qquad w_{ij} := \frac{e^2}{|\mathbf{x}_i-\mathbf{x}_j|}\,,$$

for all $i\in\{1,\dots,N\}$ and $1\leqslant i<j\leqslant N$, respectively. Thanks to [10, Proof of Lemma 3.4(ii)], which implies that $P^+_{\mathbf{A}}$ maps $\mathscr{D}$ into $\mathcal{D}(|D_{\mathbf{0}}|)\cap\mathcal{D}(H^\nu_{\mathrm{f}})$, for every $\nu>0$, and Hardy's inequality, we actually know that $H^{V_{\mathrm{C}}}_{\mathrm{np}}$ is well-defined on $\mathscr{D}_N$. In order to apply Corollary 2.3 to $H^{V_{\mathrm{C}}}_{\mathrm{np}}$ we extend $H^{V_{\mathrm{C}}}_{\mathrm{np}}$ to a continuously invertible operator on the whole space $\mathscr{H}_N$: We pick the complementary projection,

$$P^\perp_{\mathbf{A},N} := \mathbb{1} - P^+_{\mathbf{A},N}\,,$$

abbreviate

$$P^{+,(i,j)}_{\mathbf{A}} := P^{+,(i)}_{\mathbf{A}}\,P^{+,(j)}_{\mathbf{A}} = P^{+,(j)}_{\mathbf{A}}\,P^{+,(i)}_{\mathbf{A}}\,,\qquad 1\leqslant i<j\leqslant N\,,$$

and define the operator $\widetilde{H}_{\mathrm{np}}$ a priori on the domain $\mathscr{D}_N$ by

$$\widetilde{H}_{\mathrm{np}} := \sum_{i=1}^N\big\{\,|D^{(i)}_{\mathbf{A}}| + P^{+,(i)}_{\mathbf{A}}\,v_i\,P^{+,(i)}_{\mathbf{A}}\,\big\} + \sum_{\substack{i,j=1\\ i<j}}^N P^{+,(i,j)}_{\mathbf{A}}\,w_{ij}\,P^{+,(i,j)}_{\mathbf{A}}$$

$$+\,P^+_{\mathbf{A},N}\,H_{\mathrm{f}}\,P^+_{\mathbf{A},N} + P^\perp_{\mathbf{A},N}\,H_{\mathrm{f}}\,P^\perp_{\mathbf{A},N}\,. \tag{6.2}$$

Evidently, we have $[\widetilde{H}_{\mathrm{np}}\,,\,P^+_{\mathbf{A},N}]=0$ and $\widetilde{H}_{\mathrm{np}}\,P^+_{\mathbf{A},N} = H^{V_{\mathrm{C}}}_{\mathrm{np}}\,P^+_{\mathbf{A},N}$ on $\mathscr{D}_N$. In Proposition A.2 we show that the quadratic forms of the no-pair operator $H^{V_{\mathrm{C}}}_{\mathrm{np}}$ and of $\widetilde{H}_{\mathrm{np}}$ are semi-bounded below on $\mathscr{D}_N$ provided that the atomic numbers $Z_1,\dots,Z_K\geqslant 0$ are less than the critical one of the Brown-Ravenhall model determined in [3],

$$Z_{\mathrm{np}} := (2/e^2)/(2/\pi+\pi/2)\,. \tag{6.3}$$

Therefore, both $H^{V_{\mathrm{C}}}_{\mathrm{np}}$ and $\widetilde{H}_{\mathrm{np}}$ possess self-adjoint Friedrichs extensions which are again denoted by the same symbols in the sequel. $\mathscr{D}_N$ is a form core for

$\widetilde{H}_{\rm np}$ and we have the bound

$$\widetilde{H}_{\rm np}-\sum_{i=1}^{N}P_{\mathbf{A}}^{+,(i)}\,v_i\,P_{\mathbf{A}}^{+,(i)}\;\leqslant\;\frac{Z_{\rm np}+|\mathscr{Z}|}{Z_{\rm np}-|\mathscr{Z}|}\,\big(\widetilde{H}_{\rm np}+C(N,\mathscr{Z},\mathscr{R},d_{-1},d_1,d_5)\big) \tag{6.4}$$

on $\mathscr{D}_N$, where $|\mathscr{Z}|:=\max\{Z_1,\dots,Z_K\}<Z_{\rm np}$. Moreover, it makes sense to define

$$E_{\rm np}\;:=\;\inf\sigma[H_{\rm np}^{V_{\rm C}}]\,,$$

so that

$$H'_{\rm np}\;:=\;\widetilde{H}_{\rm np}-E_{\rm np}\,P_{\mathbf{A},N}^{+}+\mathbb{1}\;\geqslant\;\mathbb{1}\,.$$

Theorem 6.1. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1 and let $N,K\in\mathbb{N}$, $e>0$, $\mathscr{Z}=(Z_1,\dots,Z_K)\in[0,Z_{\rm np})^K$, and $\mathscr{R}=\{\mathbf{R}_1,\dots,\mathbf{R}_K\}\subset\mathbb{R}^3$, where $Z_{\rm np}$ is defined in* (6.3). *Then $\mathcal{D}((H'_{\rm np})^{m/2})\subset\mathcal{D}(H_{\rm f}^{m/2})$, for every $m\in\mathbb{N}$, and*

$$\begin{aligned}\big\|\,H_{\rm f}^{m/2}\!\restriction_{\mathscr{H}_N^+}(H_{\rm np}-(E_{\rm np}-1)\,\mathbb{1}_{\mathscr{H}_N^+})^{-m/2}\,\big\|_{\mathscr{L}(\mathscr{H}_N^+,\mathscr{H}_N)}&\leqslant\big\|\,H_{\rm f}^{m/2}\,(H'_{\rm np})^{-m/2}\,\big\|\\ \leqslant C(N,m,\mathscr{Z},\mathscr{R},e,d_{-1},d_1,d_{5+m})\,(1+|E_{\rm np}|)^{(3m-2)/2}&<\infty\,.\end{aligned}$$

Proof. Let $m\in\mathbb{N}$. Again we pick the function f_ε defined in (3.10) and set $F_\varepsilon:=f_\varepsilon^{1/2}(H_{\rm f})$, $\varepsilon>0$. This time we choose $E=\max\{k\,d_1^2,k_1,C\}$ where k is the constant appearing in (3.19), $C\equiv C(d_1)$ is the one in (5.3), and k_1 the one appearing in Lemma 3.3 with $|\kappa|=(m+1)/2$, $|\nu|=1/2$. Thus k_1 depends only on m, d_1, and d_{5+m}. On account of Corollary 2.3 it suffices to show that the conditions (a)–(c) of Theorem 2.1 are fulfilled. To this end we observe that on $\mathscr{D}_N$ the extended no-pair operator can be written as $H'_{\rm np}=H^0_{\rm sr}+\mathbb{1}+W$, where

$$\begin{aligned}W\;:=\;\sum_{i=1}^{N}P_{\mathbf{A}}^{+,(i)}\,v_i\,P_{\mathbf{A}}^{+,(i)}+\sum_{\substack{i,j=1\\ i<j}}^{N}P_{\mathbf{A}}^{+,(i,j)}\,w_{ij}\,P_{\mathbf{A}}^{+,(i,j)}&\\ -E_{\rm np}\,P_{\mathbf{A},N}^{+}-2\mathrm{Re}\big[P_{\mathbf{A},N}^{+}\,H_{\rm f}\,P_{\mathbf{A},N}^{\perp}\big]&\,.\end{aligned}$$

The semi-relativistic Pauli-Fierz operator $H^0_{\rm sr}$ has already been treated in the previous section and the bound

$$H_{\rm f}\;\leqslant\;2P_{\mathbf{A},N}^{+}\,H_{\rm f}\,P_{\mathbf{A},N}^{+}+2P_{\mathbf{A},N}^{\perp}\,H_{\rm f}\,P_{\mathbf{A},N}^{\perp} \tag{6.5}$$

together with (6.4) implies

$$H^0_{\rm sr}\;\leqslant\;2\,\widetilde{H}_{\rm np}-2\sum_{i=1}^{N}P_{\mathbf{A}}^{+,(i)}\,v_i\,P_{\mathbf{A}}^{+,(i)}\;\leqslant\;C'\,(1+|E_{\rm np}|)\,H'_{\rm np} \tag{6.6}$$

on $\mathscr{D}_N$, for some $C'\equiv C'(N,\mathscr{Z},\mathscr{R},d_{-1},d_1,d_5)\in(0,\infty)$. Hence, it only remains to consider the operator W.

We fix some $n \in \mathbb{N}$, $n \leqslant m$. When we verify (a) we can ignore the potentials v_i since they are negative. Using $[F_\varepsilon^n, P^\perp_{\mathbf{A},N}] = [P^+_{\mathbf{A},N}, F_\varepsilon^n]$ we obtain

$$\begin{aligned}
&\big|2\mathrm{Re}\,\big\langle\, P^+_{\mathbf{A},N}\, F_\varepsilon\, \Psi \,\big|\, H_\mathrm{f}\, P^\perp_{\mathbf{A},N}\, F_\varepsilon\, \Psi \,\big\rangle\big| \\
&\qquad \leqslant \big\|\, H_\mathrm{f}^{1/2}\, P^+_{\mathbf{A},N}\, F_\varepsilon\, \Psi \,\big\|^2 + \big\|\, H_\mathrm{f}^{1/2}\, P^\perp_{\mathbf{A},N}\, F_\varepsilon\, \Psi \,\big\|^2 \\
&\qquad \leqslant 2\,\|f_\varepsilon\|_\infty \,\big\|H_\mathrm{f}^{1/2}\, P^+_{\mathbf{A},N}\, \Psi\big\|^2 + 2\,\|f_\varepsilon\|_\infty\, \big\|H_\mathrm{f}^{1/2}\, P^\perp_{\mathbf{A},N}\, \Psi\big\|^2 \\
&\qquad\quad + 4\,\big\|\, H_\mathrm{f}^{1/2}\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon]\, \check{H}_\mathrm{f}^{-1/2} \,\big\|\, \|\check{H}_\mathrm{f}^{1/2}\, \Psi\|^2,
\end{aligned}$$

for every $\Psi \in \mathscr{D}_N$, where, for all $n \in \mathbb{N}$ and $\nu \in \mathbb{R}$,

$$\begin{aligned}
\check{H}_\mathrm{f}^\nu\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon^n]\, \check{H}_\mathrm{f}^{-\nu}\, F_\varepsilon^{1-n} \;&=\; \sum_{i=1}^N \Big\{ \prod_{j=1}^{i-1} \check{H}_\mathrm{f}^\nu\, P_{\mathbf{A}}^{+,(j)}\, \check{H}_\mathrm{f}^{-\nu} \Big\} \times \\
\times\; \big\{ \check{H}_\mathrm{f}^\nu\, [P_{\mathbf{A}}^{+,(i)}, F_\varepsilon^n]\, \check{H}_\mathrm{f}^{-\nu}\, F_\varepsilon^{1-n} \big\}&\Big\{ \prod_{k=i+1}^N \check{H}_\mathrm{f}^\nu\, F_\varepsilon^{n-1}\, P_{\mathbf{A}}^{+,(k)}\, \check{H}_\mathrm{f}^{-\nu}\, F_\varepsilon^{1-n} \Big\}
\end{aligned}$$

on $\mathscr{D}_N$. On account of Corollary 3.4 we thus have, for $|\nu| \leqslant 1/2$,

$$\sup_{\varepsilon>0} \big\|\, H_\mathrm{f}^\nu\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon^n]\, \check{H}_\mathrm{f}^{-\nu}\, F_\varepsilon^{1-n} \,\big\| \;\leqslant\; C(N, n, d_1, d_{4+n})\,. \tag{6.7}$$

Likewise we have

$$\begin{aligned}
\big|\big\langle\, F_\varepsilon\, \Psi \,\big|\, P_{\mathbf{A}}^{+,(i,j)}\, w_{ij}\, P_{\mathbf{A}}^{+,(i,j)}\, F_\varepsilon\, \Psi \,\big\rangle\big| \;&\leqslant\; 2\,\|f_\varepsilon\|\, \big\|\, w_{ij}^{1/2}\, P_{\mathbf{A}}^{+,(i,j)}\, \Psi \,\big\|^2 \\
&\quad + 4\,\big\|\, w_{ij}^{1/2}\, [P_{\mathbf{A}}^{+,(i,j)}\,,\, F_\varepsilon]\, \check{H}_\mathrm{f}^{-1/2} \,\big\|^2\, \|\check{H}_\mathrm{f}^{1/2}\, \Psi\|^2,
\end{aligned} \tag{6.8}$$

where the first norm in the second line of (6.8) is bounded (uniformly in $\varepsilon > 0$) due to Lemma 6.2. Taking these remarks, $v_i \leqslant 0$, (6.4), and (6.5) into account we infer that

$$\big\langle\, F_\varepsilon\, \Psi \,\big|\, H'_\mathrm{np}\, F_\varepsilon\, \Psi \,\big\rangle \;\leqslant\; c_\varepsilon \big\langle\, \Psi \,\big|\, H'_\mathrm{np}\, \Psi \,\big\rangle\,, \qquad \Psi \in \mathscr{D}_N\,,$$

showing that (a) is fulfilled. The condition (b) with some constant $c^2 = C(N, \mathscr{Z}, \mathscr{R}, d_{-1}, d_1, d_5)(1+|E_\mathrm{np}|)$ follows immediately from $F_\varepsilon^2 \leqslant \check{H}_\mathrm{f} \leqslant H^0_\mathrm{sr} + E$ on $\mathscr{D}_N$ and (6.6). Finally, we turn to Condition (c). To this end let $P^\sharp_{\mathbf{A},N}$ and $P^\flat_{\mathbf{A},N}$ be $P^+_{\mathbf{A},N}$ or $P^\perp_{\mathbf{A},N}$. On $\mathscr{D}_N$ we clearly have

$$\big[\, P^\sharp_{\mathbf{A},N}\, H_\mathrm{f}\, P^\flat_{\mathbf{A},N}\,,\, F_\varepsilon^n \,\big] \;=\; \pm\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon^n]\, H_\mathrm{f}\, P^\flat_{\mathbf{A},N} \;\pm\; P^\sharp_{\mathbf{A},N}\, H_\mathrm{f}\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon^n]\,. \tag{6.9}$$

For $\Psi_1, \Psi_2 \in \mathscr{D}_N$, we thus obtain

$$\begin{aligned}
&\big|\big\langle\, \Psi_1 \,\big|\, \big[\, P^\sharp_{\mathbf{A},N}\, H_\mathrm{f}\, P^\flat_{\mathbf{A},N}\,,\, F_\varepsilon^n \,\big]\, \Psi_2 \,\big\rangle\big| \\
&\qquad \leqslant \|\check{H}_\mathrm{f}^{1/2}\, \Psi_1\|\, \big\|\, \check{H}_\mathrm{f}^{-1/2}\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon^n]\, H_\mathrm{f}^{1/2} F^{1-n} \,\big\|\, \big\|H_\mathrm{f}^{1/2}\, F_\varepsilon^{n-1}\, P^\flat_{\mathbf{A},N}\, \Psi_2\big\| \\
&\qquad + \|H_\mathrm{f}^{1/2}\, P^\sharp_{\mathbf{A},N}\, \Psi_1\|\, \big\|H_\mathrm{f}^{1/2}\, [P^+_{\mathbf{A},N}\,,\, F_\varepsilon^n]\, \check{H}_\mathrm{f}^{-1/2}\, F_\varepsilon^{1-n}\big\|\, \|\check{H}_\mathrm{f}^{1/2}\, F_\varepsilon^{n-1}\, \Psi_2\|\,,
\end{aligned} \tag{6.10}$$

where we can further estimate

$$\begin{aligned}&\big\|H_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,P^\flat_{\mathbf{A},N}\,\Psi_2\big\|\\ &\qquad\leqslant\big\{1+\big\|H_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,P^+_{\mathbf{A},N}\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{1-n}\big\|\big\}\,\|\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|\\ &\qquad\leqslant\big\{1+\|H_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,P^+_{\mathbf{A}}\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{1-n}\|^N\big\}\,\|\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|\,,\end{aligned}\tag{6.11}$$

and, of course,

$$\|\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|\leqslant\|\check{H}_{\mathrm{f}}^{1/2}\,P^+_{\mathbf{A},N}\,F_\varepsilon^{n-1}\,\Psi_2\|+\|\check{H}_{\mathrm{f}}^{1/2}\,P^\perp_{\mathbf{A},N}\,F_\varepsilon^{n-1}\,\Psi_2\|\,.\tag{6.12}$$

The operator norms in (6.10) can be estimated by means of (6.7) with $\nu=\pm1/2$, the one in the last line of (6.11) is bounded by some $C(n,d_1,d_{3+n})\in(0,\infty)$ due to (3.21). In a similar fashion we obtain, for all $i,j\in\{1,\dots,N\}$, $i<j$, and $\Psi_1,\Psi_2\in\mathscr{D}_N$,

$$\begin{aligned}&\big|\big\langle\,\Psi_1\,\big|\,[P_{\mathbf{A}}^{+,(i,j)}\,w_{ij}P_{\mathbf{A}}^{+,(i,j)}\,,\,F_\varepsilon^n]\,\Psi_2\,\big\rangle\big|\\ &\leqslant\big\|\,F_\varepsilon^{1-n}\,w_{ij}^{1/2}\,[F_\varepsilon^n\,,\,P_{\mathbf{A}}^{+,(i,j)}]\,\check{H}_{\mathrm{f}}^{-1/2}\,\big\|\,\|\check{H}_{\mathrm{f}}^{1/2}\,\Psi_1\|\,\big\|F_\varepsilon^{n-1}\,w_{ij}^{1/2}\,P_{\mathbf{A}}^{+,(i,j)}\,\Psi_2\big\|\\ &\quad+\big\|\,w_{ij}^{1/2}\,P_{\mathbf{A}}^{+,(i,j)}\,\Psi_1\big\|\,\big\|\,w_{ij}^{1/2}\,[P_{\mathbf{A}}^{+,(i,j)},\,F_\varepsilon^n]\,F_\varepsilon^{1-n}\,\check{H}_{\mathrm{f}}^{-1/2}\big\|\,\|\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|.\end{aligned}\tag{6.13}$$

Here we can further estimate

$$\begin{aligned}\big\|\,w_{ij}^{1/2}\,F_\varepsilon^{n-1}\,P_{\mathbf{A}}^{+,(i,j)}\,\Psi_2\big\|&\leqslant\big\|\,w_{ij}^{1/2}\,P_{\mathbf{A}}^{+,(i,j)}\,F_\varepsilon^{n-1}\,\Psi_2\big\|\\ &\quad+\big\|\,w_{ij}^{1/2}\,[F_\varepsilon^{n-1}\,,\,P_{\mathbf{A}}^{+,(i,j)}]\,\check{H}_{\mathrm{f}}^{-1/2}F_\varepsilon^{1-n}\,\big\|\,\|\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^{n-1}\,\Psi_2\|\,.\end{aligned}\tag{6.14}$$

Lemma 6.2 below ensures that all operator norms in (6.13) and (6.14) that involve $w_{ij}^{1/2}$ are bounded uniformly in $\varepsilon>0$ by constants depending only on e,n,d_1, and d_{5+n}. Furthermore, it is now clear how to treat the terms involving v_i or E_{np}. (In order to treat v_i just replace $P_{\mathbf{A}}^{+,(i,j)}$ by $P_{\mathbf{A}}^{+,(i)}$, w_{ij} by v_i, and $w_{ij}^{1/2}$ by $|v_i|^{1/2}$ in (6.13) and (6.14).) Combining (6.9)–(6.14) and their analogues for the remaining operators in W we arrive at

$$\begin{aligned}&\big|\big\langle\,\Psi_1\,\big|\,[W\,,\,F_\varepsilon^n]\,\Psi_2\,\big\rangle\big|\\ &\leqslant C\sum_{\sharp\in\{+,\perp\}}\big\{\big\langle\,\Psi_1\,\big|\,P^\sharp_{\mathbf{A},N}\,H_{\mathrm{f}}\,P^\sharp_{\mathbf{A},N}\,\Psi_1\,\big\rangle+\big\langle\,F_\varepsilon^{n-1}\,\Psi_2\,\big|\,P^\sharp_{\mathbf{A},N}\,H_{\mathrm{f}}\,P^\sharp_{\mathbf{A},N}\,F_\varepsilon^{n-1}\,\Psi_2\,\big\rangle\big\}\\ &+C\sum_{\substack{i,j=1\\ i<j}}^N\big\{\big\langle\,\Psi_1\,\big|\,P_{\mathbf{A}}^{+,(i,j)}w_{ij}P_{\mathbf{A}}^{+,(i,j)}\Psi_1\,\big\rangle\\ &\qquad\qquad+\big\langle\,F_\varepsilon^{n-1}\Psi_2\,\big|\,P_{\mathbf{A}}^{+,(i,j)}w_{ij}P_{\mathbf{A}}^{+,(i,j)}F_\varepsilon^{n-1}\Psi_2\,\big\rangle\big\}\\ &+C\sum_{i=1}^N\big\{\big\langle\,\Psi_1\,\big|\,P_{\mathbf{A}}^{+,(i)}\,|v_i|\,P_{\mathbf{A}}^{+,(i)}\,\Psi_1\,\big\rangle+\big\langle\,F_\varepsilon^{n-1}\,\Psi_2\,\big|\,P_{\mathbf{A}}^{+,(i)}\,|v_i|\,P_{\mathbf{A}}^{+,(i)}\,F_\varepsilon^{n-1}\,\Psi_2\,\big\rangle\big\}\\ &+C\,(1+|E_{\mathrm{np}}|)\,\big\{\|\Psi_1\|^2+\|F_\varepsilon^{n-1}\,\Psi_2\|^2\big\}\,,\end{aligned}$$

for all $\Psi_1,\Psi_2\in\mathscr{D}_N$ and some ε-independent $C\equiv C(N,n,e,d_1,d_{5+n})\in(0,\infty)$. Employing successively (3.19), which implies $|v_i|\leqslant(\pi e^2|\mathscr{Z}|/2)(|D_{\mathbf{A}}^{(i)}|+\check{H}_{\mathrm{f}})$, after that (3.21), which yields $\|\check{H}_{\mathrm{f}}^{1/2}\, P^{+,(i)}_{\mathbf{A}}\, \Psi\|^2 \leqslant C(d_1,d_4)(\|\check{H}_{\mathrm{f}}^{1/2}\, P^{+}_{\mathbf{A},N}\, \Psi\|^2 + \|\check{H}_{\mathrm{f}}^{1/2}\, P^{\perp}_{\mathbf{A},N}\, \Psi\|^2)$, and finally (6.4) we conclude that Condition (c) is fulfilled with $c_n = C(N,n,\mathscr{Z},\mathscr{R},e,d_{-1},d_1,d_{5+n})(1+|E_{\mathrm{np}}|)$. □

Lemma 6.2. *For all $i,j \in \{1,\dots,N\}$, $i<j$, $n\in\mathbb{Z}$, and $\sigma,\tau \geqslant 0$ with $\sigma+\tau\leqslant 1$,*

$$\sup_{\varepsilon>0}\big\|F_\varepsilon^{\sigma-n}\, w_{ij}^{1/2}\,[F_\varepsilon^n\,,\,P^{+,(i,j)}_{\mathbf{A}}]\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^\tau\,\big\|$$

$$= \sup_{\varepsilon>0}\big\|\,w_{ij}^{1/2}\,F_\varepsilon^\sigma\,[P^{+,(i,j)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{n+\tau}\,\big\| \,\leqslant\, e\,C(n,d_1,d_{5+n}) \,<\, \infty\,.$$

Proof. We write

$$w_{ij}^{1/2}\,F_\varepsilon^\sigma\,[P^{+,(i)}_{\mathbf{A}}\,P^{+,(j)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,\check{H}_{\mathrm{f}}^{-1/2}F_\varepsilon^{n+\tau} \,=\, Y_1 + w_{ij}^{1/2}\,Y_2 + Y_3\,,$$

where

$$Y_1 := \{w_{ij}^{1/2}\,F_\varepsilon^\sigma\,[P^{+,(i)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{n+\tau}\}\{\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^{-n-\tau}\,P^{+,(j)}_{\mathbf{A}}\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{n+\tau}\},$$

$$Y_2 := P^{+,(i)}_{\mathbf{A}}\,F_\varepsilon^\sigma\,[P^{+,(j)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{n+\tau},$$

$$Y_3 := w_{ij}^{1/2}\,[F_\varepsilon^\sigma\,,\,P^{+,(i)}_{\mathbf{A}}]\,[P^{+,(j)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{n+\tau}.$$

Applying Corollary 3.4 we immediately see that $\|Y_1\| \leqslant e\,C(n,d_1,d_{5+n})$ and that

$$\|Y_3\| \leqslant \big\|\,w_{ij}^{1/2}\,[F_\varepsilon^\sigma\,,\,P^{+,(i)}_{\mathbf{A}}]\,F_\varepsilon^{-\sigma}\big\|\,\big\|\,F_\varepsilon^\sigma\,[P^{+,(j)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,F_\varepsilon^{n+\tau}\,\big\| \leqslant e\,C(n,d_1,d_{3+n})$$

uniformly in $\varepsilon>0$. Employing (3.19) (with respect to the variable $\mathbf{x}_j$ for each fixed $\mathbf{x}_i$) and using $[|D^{(j)}_{\mathbf{A}}|^{1/2}, P^{+,(i)}_{\mathbf{A}}] = 0$, we further get

$$\begin{aligned}
&\big\|\,w_{ij}^{1/2}\,Y_2\,\Psi\big\|^2\\
&\leqslant\, (\pi e^2/2)\,\|P^{+,(i)}_{\mathbf{A}}\|^2\,\big\|\,|D^{(j)}_{\mathbf{A}}|^{1/2}\,F_\varepsilon^\sigma\,[P^{+,(j)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,F_\varepsilon^{n+\tau}\big\|^2\,\|\check{H}_{\mathrm{f}}^{-1/2}\|^2\\
&\quad+ (\pi e^2/2)\,\big\|\check{H}_{\mathrm{f}}^{1/2}\,P^{+,(i)}_{\mathbf{A}}\,\check{H}_{\mathrm{f}}^{-1/2}\big\|^2\,\big\|\check{H}_{\mathrm{f}}^{1/2}\,F_\varepsilon^\sigma\,[P^{+,(i)}_{\mathbf{A}}\,,\,F_\varepsilon^{-n}]\,\check{H}_{\mathrm{f}}^{-1/2}\,F_\varepsilon^{n+\tau}\big\|^2.
\end{aligned}$$

By Corollary 3.4 all norms on the right hand side are bounded uniformly in $\varepsilon>0$ by constants depending only on n, d_1, and d_{4+n}. □

Appendix A. Semi-boundedness of $H^{V_{\mathrm{C}}}_{\mathrm{sr}}$ and $H^{V_{\mathrm{C}}}_{\mathrm{np}}$

In this appendix we verify that the semi-relativistic Pauli-Fierz and no-pair operators with Coulomb potential are semi-bounded below for all nuclear charges less than the critical charges without radiation fields. We do not attempt to give good lower bounds on their spectra since this is not the topic addressed in this paper. Our aim here is essentially only to ensure that these operators possess self-adjoint Friedrichs extensions. We recall that the stability of matter of the second kind has been proven for the no-pair operator in [9] under certain restrictions on the fine-structure constant, the ultra-violet cut-off, and the nuclear charges. The stability of matter of the second kind is a much stronger property than mere semi-boundedness. It says that the operator is bounded below by some constant which is proportional to the total number of nuclei and electrons and uniform in the nuclear positions. The restrictions imposed

on the physical parameters in [9] do, however, not allow for all atomic numbers less than Z_{np}.
First, we consider the semi-relativistic Pauli-Fierz operator. The following proposition is a simple generalization of the bound (3.19) proven in [10] to the case of $N \in \mathbb{N}$ electrons and $K \in \mathbb{N}$ nuclei.

Proposition A.1. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1 and let $N, K \in \mathbb{N}$, $e > 0$, $\mathscr{Z} = (Z_1, \dots, Z_K) \in (0, 2/\pi e^2]^K$, and $\mathscr{R} = \{\mathbf{R}_1, \dots, \mathbf{R}_K\} \subset \mathbb{R}^3$. Then*

$$\sum_{i=1}^{N} |D_{\mathbf{A}}^{(i)}| + V_{\mathrm{C}} + \delta\, H_{\mathrm{f}} \geqslant -C(\delta, N, \mathscr{Z}, \mathscr{R}, d_1) > -\infty\,, \tag{A.1}$$

for every $\delta > 0$ in the sense of quadratic forms on $\mathscr{D}_N$.

Proof. In view of (3.19) we only have to explain how to localize the non-local kinetic energy terms. To begin with we recall the following bounds proven in [10, Lemmata 3.5 and 3.6]: For every $\chi \in C^\infty(\mathbb{R}^3_{\mathbf{x}}, [0,1])$,

$$\| [\chi, S_{\mathbf{A}}] \| \leqslant \|\nabla \chi\|_\infty\,, \qquad \big\| D_{\mathbf{A}} \big[\chi\,,\, [\chi, S_{\mathbf{A}}]\big] \big\| \leqslant 2\, \|\nabla \chi\|_\infty^2\,. \tag{A.2}$$

Now, let $\mathcal{B}_r(\mathbf{z})$ denote the open ball of radius $r > 0$ centered at $\mathbf{z} \in \mathbb{R}^3$ in $\mathbb{R}^3$. We set $\varrho := \min\{|\mathbf{R}_k - \mathbf{R}_\ell| : k \neq \ell\}/2$ and pick a smooth partition of unity on $\mathbb{R}^3$, $\{\chi_k\}_{k=0}^K$, such that $\chi_k \equiv 1$ on $\mathcal{B}_{\varrho/2}(\mathbf{R}_k)$ and $\mathrm{supp}(\chi_k) \subset \mathcal{B}_\varrho(\mathbf{R}_k)$, for $k = 1, \dots, K$, and such that $\sum_{k=0}^K \chi_k^2 = 1$. Then we have the following IMS type localization formula,

$$|D_{\mathbf{A}}| = \sum_{k=0}^{K} \Big\{ \chi_k\, |D_{\mathbf{A}}|\, \chi_k + \frac{1}{2} \big[\chi_k\,,\, [\chi_k, |D_{\mathbf{A}}|\,]\big] \Big\} \tag{A.3}$$

on $\mathscr{D}$, for every $i \in \{1, \dots, N\}$. A direct calculation shows that

$$\big[\chi_k\,,\, [\chi_k, |D_{\mathbf{A}}|\,]\big] = 2\, i \boldsymbol{\alpha} \cdot (\nabla \chi_k)\, [\chi_k, S_{\mathbf{A}}] + D_{\mathbf{A}} \big[\chi_k\,,\, [\chi_k, S_{\mathbf{A}}]\big] \tag{A.4}$$

on $\mathscr{D}$. By virtue of (3.6) and (A.2) we thus get

$$\big\| \big[\chi_k\,,\, [\chi_k, |D_{\mathbf{A}}|\,]\big] \big\| \leqslant 4\, \|\nabla \chi\|_\infty^2\,, \tag{A.5}$$

for all $k \in \{0, \dots, K\}$. Since we are able to localize the kinetic energy terms and since, by the choice of the partition of unity, the functions $\mathbb{R}^3 \ni \mathbf{x} \mapsto |\mathbf{x} - \mathbf{R}_k|^{-1}\, \chi_\ell^2(\mathbf{x})$ are bounded, for $k \in \{1, \dots, K\}$, $\ell \in \{0, \dots, K\}$, $k \neq \ell$, the bound (A.1) is now an immediate consequence of (3.19) (with δ replaced by δ/N). (Here we also make use of the fact that the hypotheses on $\mathbf{G}$ are translation invariant.) □

Next, we turn to the no-pair operator discussed in Section 6. The semi-boundedness of the molecular N-electron no-pair operator is essentially a consequence of the following inequality [10, Equation (2.14)], valid for all ω and $\mathbf{G}$ fulfilling Hypothesis 3.1, $\gamma \in (0, 2/(2/\pi + \pi/2))$, and $\delta > 0$,

$$P_{\mathbf{A}}^+ \, (D_{\mathbf{A}}^{(i)} - \gamma/|\mathbf{x}| + \delta\, H_{\mathrm{f}})\, P_{\mathbf{A}}^+ \geqslant P_{\mathbf{A}}^+ \, (c(\gamma)\, |D_{\mathbf{0}}| - C)\, P_{\mathbf{A}}^+\,, \tag{A.6}$$

in the sense of quadratic forms on $P^+_{\mathbf{A}}\,\mathscr{D}$. Here $C \equiv C(\delta,\gamma,d_{-1},d_0,d_1) \in (0,\infty)$ and $c(\gamma) \in (0,\infty)$ depends only on γ.

Proposition A.2. *Assume that ω and $\mathbf{G}$ fulfill Hypothesis 3.1 and let $N, K \in \mathbb{N}$, $e > 0$, $\mathscr{Z} = (Z_1,\ldots,Z_K) \in (0,Z_{\mathrm{np}})^K$, and $\mathscr{R} = \{\mathbf{R}_1,\ldots,\mathbf{R}_K\} \subset \mathbb{R}^3$, where Z_{np} is defined in* (6.3). *Then the quadratic form associated with the operator $\widetilde{H}_{\mathrm{np}}$ defined in* (6.2) *is semi-bounded below,*

$$\widetilde{H}_{\mathrm{np}} \,\geqslant\, -C(N,K,\mathscr{Z},\mathscr{R},d_{-1},d_1,d_5) \,>\, -\infty\,,$$

in the sense of quadratic forms on $\mathscr{D}_N$.

Proof. We again employ the parameter $\varrho > 0$ and the partition of unity introduced in the paragraph succeeding (A.2). Thanks to [10, Proof of Lemma 3.4(ii)] we know that $P^+_{\mathbf{A}}$ maps $\mathcal{D}(D_{\mathbf{0}} \otimes H_{\mathrm{f}}^{\nu})$ into $\mathcal{D}(D_{\mathbf{0}} \otimes H_{\mathrm{f}}^{\nu-1})$, for every $\nu \geqslant 1$. The IMS localization formula thus yields

$$\begin{aligned} &P^{+,(i)}_{\mathbf{A}}\, v_i\, P^{+,(i)}_{\mathbf{A}} \\ &\quad= \sum_{k=0}^{K} \Big\{ \chi^{(i)}_k\, P^{+,(i)}_{\mathbf{A}}\, v_i\, P^{+,(i)}_{\mathbf{A}}\, \chi^{(i)}_k \,+\, \frac{1}{2}\,\big[\chi^{(i)}_k\,,\,[\chi^{(i)}_k\,,\,P^{+,(i)}_{\mathbf{A}}\, v_i\, P^{+,(i)}_{\mathbf{A}}]\,\big]\Big\} \end{aligned}$$

on $\mathcal{D}(D_{\mathbf{0}} \otimes H_{\mathrm{f}})$, where a superscript (i) indicates that $\chi_k = \chi_k^{(i)}$ depends on the variable $\mathbf{x}_i$. Using $v_i \leqslant 0$, we observe that

$$\begin{aligned} &\big[\chi^{(i)}_k\,,\,[\chi^{(i)}_k\,,\,P^{+,(i)}_{\mathbf{A}}\, v_i\, P^{+,(i)}_{\mathbf{A}}]\,\big] \\ &\quad= -2\,[\chi^{(i)}_k\,,\,P^{+,(i)}_{\mathbf{A}}]\, v_i\, [P^{+,(i)}_{\mathbf{A}}\,,\,\chi^{(i)}_k] \\ &\qquad + 2\,\mathrm{Re}\,\big\{\, P^{+,(i)}_{\mathbf{A}}\, v_i\, \big[\chi^{(i)}_k\,,\,[\chi^{(i)}_k\,,\,P^{+,(i)}_{\mathbf{A}}]\,\big]\,\big\} \\ &\quad\geqslant\, 2\,\mathrm{Re}\,\big\{\, P^{+,(i)}_{\mathbf{A}}\, v_i\, \big[\chi^{(i)}_k\,,\,[\chi^{(i)}_k\,,\,P^{+,(i)}_{\mathbf{A}}]\,\big]\,\big\}\,. \end{aligned} \tag{A.7}$$

We recall the following estimate proven in [10, Lemma 3.6], for every $\chi \in C^\infty(\mathbb{R}^3_{\mathbf{x}},[0,1])$,

$$\big\|\tfrac{1}{|\mathbf{x}|}\,\big[\chi\,,\,[\chi\,,\,P^+_{\mathbf{A}}]\,\big]\,\check{H}_{\mathrm{f}}^{-1/2}\,\big\| \,\leqslant\, 8^{3/2}\,\|\nabla\chi\|^2_\infty\,,$$

where $\check{H}_{\mathrm{f}} = H_{\mathrm{f}} + E$ with $E \geqslant 1 \vee (4d_1)^2$. Together with (A.7) it implies

$$\begin{aligned} &\big\langle\, \Psi\,\big|\,\big[\chi^{(i)}_k\,,[\chi^{(i)}_k\,,\,P^{+,(i)}_{\mathbf{A}}\, v_i\, P^{+,(i)}_{\mathbf{A}}]\,\big]\,\Psi\,\big\rangle \\ &\qquad\geqslant\, -\delta\,\langle\,\Psi\,|\,\check{H}_{\mathrm{f}}\,\Psi\,\rangle - (8^3\,\|\nabla\chi_k\|^4_\infty/\delta)\,\|\Psi\|^2, \end{aligned}$$

for all $k \in \{0,\ldots,K\}$, $i \in \{1,\ldots,N\}$, $\delta > 0$, and $\Psi \in \mathcal{D}(D_{\mathbf{0}} \otimes H_{\mathrm{f}})$. Next, we pick cut-off functions, $\zeta_1,\ldots,\zeta_K \in C_0^\infty(\mathbb{R}^3_{\mathbf{x}},[0,1])$, such that $\zeta_k = 1$ in a neighborhood of $\mathbf{R}_k$ and $\mathrm{supp}(\zeta_k) \subset \mathcal{B}_{\varrho/4}(\mathbf{R}_k)$, for $k \in \{1,\ldots,K\}$. By construction, $\mathrm{supp}(\zeta_k) \cap \mathrm{supp}(\chi_\ell) = \varnothing$, for all $k \in \{1,\ldots,K\}$ and $\ell \in \{0,\ldots,K\}$ with $k \neq \ell$. Denoting $\overline{\zeta}_k := 1 - \zeta_k$ and using the superscript (i) to indicate that $\zeta_k = \zeta_k^{(i)}$

is a function of the variable $\mathbf{x}_i$, we obtain

$$\begin{aligned}\big\langle\,\Psi\,\big|\,\chi_k^{(i)}\,P_{\mathbf{A}}^{+,(i)}\,v_i\,P_{\mathbf{A}}^{+,(i)}\,\chi_k^{(i)}\,\Psi\,\big\rangle\\ &= -\Big\langle\,\Psi\,\Big|\,\chi_k^{(i)}\,P_{\mathbf{A}}^{+,(i)}\,\frac{e^2\,Z_k}{|\mathbf{x}_i-\mathbf{R}_k|}\,P_{\mathbf{A}}^{+,(i)}\,\chi_k^{(i)}\,\Psi\,\Big\rangle\\ \text{(A.8)}\qquad &\quad-\sum_{\substack{\ell=1\\ \ell\neq k}}^{K}\Big\langle\,\Psi\,\Big|\,\chi_k^{(i)}\,P_{\mathbf{A}}^{+,(i)}\,\frac{e^2\,Z_\ell\,\zeta_\ell^{(i)}}{|\mathbf{x}_i-\mathbf{R}_\ell|}\,P_{\mathbf{A}}^{+,(i)}\,\chi_k^{(i)}\,\Psi\,\Big\rangle\\ \text{(A.9)}\qquad &\quad-\sum_{\substack{\ell=1\\ \ell\neq k}}^{K}\Big\langle\,\Psi\,\Big|\,\chi_k^{(i)}\,P_{\mathbf{A}}^{+,(i)}\,\frac{e^2\,Z_\ell\,\overline{\zeta}_\ell^{(i)}}{|\mathbf{x}_i-\mathbf{R}_\ell|}\,P_{\mathbf{A}}^{+,(i)}\,\chi_k^{(i)}\,\Psi\,\Big\rangle,\end{aligned}$$

for all $\Psi\in\mathcal{D}(D_{\mathbf{0}}\otimes H_{\mathrm{f}})$. The operators appearing in the scalar products in (A.9) are bounded by definition of $\overline{\zeta}_\ell$. Their norms depend only on $\mathscr{R}$ since $e^2\,Z_\ell<1$. Furthermore, by virtue of Lemma A.3 below the term in (A.8) is bounded from below by $-\delta\,\langle\,\Psi\,|\,H_{\mathrm{f}}\,\Psi\,\rangle-C_\delta\,\|\Psi\|^2$, for all $\delta>0$ and some $C_\delta\equiv C_\delta(\mathscr{R},d_1,d_4)\in(0,\infty)$; see (A.11).
Taking all the previous remarks into account, using (A.3)–(A.5), $w_{ij}\geqslant 0$, $|D_{\mathbf{A}}^{(i)}|\geqslant P_{\mathbf{A}}^{+,(i)}\,D_{\mathbf{A}}^{(i)}\,P_{\mathbf{A}}^{+,(i)}$, and writing

$$H_{\mathrm{f}}\,=\,\frac{1}{N}\sum_{i=1}^{N}\sum_{k=0}^{K}\chi_k^{(i)}\,(P_{\mathbf{A}}^{+,(i)}+P_{\mathbf{A}}^{-,(i)})\,H_{\mathrm{f}}\,\chi_k^{(i)}\,,$$

we deduce that

$$\begin{aligned}&\widetilde{H}_{\mathrm{np}}\\ &\geqslant(1-3\delta)\,P_{\mathbf{A},N}^{+}\,H_{\mathrm{f}}\,P_{\mathbf{A},N}^{+}\,+\,(1-3\delta)\,P_{\mathbf{A},N}^{\perp}\,H_{\mathrm{f}}\,P_{\mathbf{A},N}^{\perp}\\ &+\sum_{\sharp\in\{+,\perp\}}\sum_{k=0}^{K}P_{\mathbf{A},N}^{\sharp}\Big\{\sum_{i=1}^{N}\chi_k^{(i)}\,P_{\mathbf{A}}^{+,(i)}\Big(D_{\mathbf{A}}^{(i)}-\frac{e^2\,Z_k}{|\mathbf{x}_i-\mathbf{R}_k|}+\frac{\delta}{N}\,H_{\mathrm{f}}\Big)\,P_{\mathbf{A}}^{+,(i)}\,\chi_k^{(i)}\\ &+\frac{\delta}{N}\sum_{i=1}^{N}\Big(\chi_k^{(i)}\,P_{\mathbf{A}}^{-,(i)}\,H_{\mathrm{f}}\,P_{\mathbf{A}}^{-,(i)}\,\chi_k^{(i)}+\sum_{\flat=\pm}\chi_k^{(i)}P_{\mathbf{A}}^{\flat,(i)}\,[P_{\mathbf{A}}^{\flat,(i)},H_{\mathrm{f}}]\,\chi_k^{(i)}\Big)\Big\}\,P_{\mathbf{A},N}^{\sharp}\\ &-\,\mathrm{const}(N,\mathscr{R},d_1,d_4)\end{aligned}$$

on $\mathscr{D}_N$, for every $\delta>0$. Thanks to Corollary 3.4 (with $\varepsilon=0$) we know that $[P_{\mathbf{A}}^{\flat,(i)},H_{\mathrm{f}}]\,\check{H}_{\mathrm{f}}^{-1/2}$ extends to an element of $\mathscr{L}(\mathscr{H}_N)$ whose norm is bounded by some constant depending only on d_1 and d_5, whence

$$\begin{aligned}&\frac{\delta}{N}\sum_{i=1}^{N}\sum_{k=0}^{K}\big\langle\,\chi_k^{(i)}\,P_{\mathbf{A},N}^{\sharp}\,\Psi\,\big|\,P_{\mathbf{A}}^{\flat,(i)}\,[P_{\mathbf{A}}^{\flat,(i)},H_{\mathrm{f}}]\,\chi_k^{(i)}\,P_{\mathbf{A},N}^{\sharp}\,\Psi\,\big\rangle\\ &\qquad\geqslant\,-(\delta/2)\,\|\check{H}_{\mathrm{f}}^{1/2}\,P_{\mathbf{A},N}^{\sharp}\,\Psi\|^2-(\delta/2)\,\big\|[P_{\mathbf{A}}^{\flat,(i)},H_{\mathrm{f}}]\check{H}_{\mathrm{f}}^{-1/2}\big\|^2\,\|\Psi\|^2,\end{aligned}$$

for every $\Psi\in\mathscr{D}_N$, $\sharp\in\{+,\perp\}$, and $\flat=\pm$. For a sufficiently small choice of $\delta>0$, the assertion of the proposition now follows from the semi-boundedness of $P_{\mathbf{A}}^{+,(i)}\,(D_{\mathbf{A}}^{(i)} - e^2\,Z_k/|\mathbf{x}_i - \mathbf{R}_k| + (\delta/N)\,H_{\mathrm{f}})\,P_{\mathbf{A}}^{+,(i)}$ ensured by (A.6) and the condition $Z_k < Z_{\mathrm{np}}$. □

LEMMA A.3. *Let* $\zeta \in C_0^\infty(\mathbb{R}^3,[0,1])$, $\chi \in C^\infty(\mathbb{R}^3,[0,1])$, *such that* $0 \in \mathrm{supp}(\zeta)$ *and* $\mathrm{supp}(\zeta) \cap \mathrm{supp}(\chi) = \varnothing$. *Set* $\check{H}_{\mathrm{f}} := H_{\mathrm{f}} + E$, *where* $E \geqslant k_1 \vee d_1^2$. *Then*

$$\big\|\, D_{\mathbf{A}}\, H_{\mathrm{f}}^{1/2}\, \zeta\, P_{\mathbf{A}}^{+}\, \chi\, \check{H}_{\mathrm{f}}^{-1/2}\,\big\| \,\leqslant\, C(\zeta,\chi,d_1,d_4)\,, \tag{A.10}$$

$$\big\|\, \tfrac{\zeta}{|\mathbf{x}|}\, P_{\mathbf{A}}^{+}\, \chi\, \check{H}_{\mathrm{f}}^{-1/2}\,\big\| \,\leqslant\, C'(\zeta,\chi,d_1,d_4)\,. \tag{A.11}$$

Proof. We pick some $\widetilde{\chi} \in C^\infty(\mathbb{R}^3,[0,1])$ such that $\mathrm{supp}(\widetilde{\chi}) \cap \mathrm{supp}(\zeta) = \varnothing$ and $\widetilde{\chi} \equiv 1$ on $\mathrm{supp}(\nabla\chi)$. Using $\zeta\,\chi = 0 = \zeta\,\widetilde{\chi}$ we infer that, for all $\varphi,\psi \in \mathscr{D}$,

$$\begin{aligned}
&\big|\big\langle\, D_{\mathbf{A}}\,\varphi \,\big|\, H_{\mathrm{f}}^{1/2}\,\zeta\,P_{\mathbf{A}}^{+}\,\chi\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\big\rangle\big| \;=\; \big|\big\langle\, D_{\mathbf{A}}\,\varphi \,\big|\, H_{\mathrm{f}}^{1/2}\,\zeta\,[P_{\mathbf{A}}^{+}\,,\,\chi]\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\big\rangle\big| \\
&\quad\leqslant \int_{\mathbb{R}} \Big|\Big\langle\, D_{\mathbf{A}}\,\varphi \,\Big|\, H_{\mathrm{f}}^{1/2}\,\zeta\,[R_{\mathbf{A}}(iy)\,,\,\widetilde{\chi}]\,i\boldsymbol{\alpha}\cdot\nabla\chi\,R_{\mathbf{A}}(iy)\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\Big\rangle\Big|\frac{dy}{2\pi} \\
&\quad= \int_{\mathbb{R}} \Big|\Big\langle\, D_{\mathbf{A}}\,\varphi \,\Big|\, H_{\mathrm{f}}^{1/2}\,\zeta\,R_{\mathbf{A}}(iy)\,i\boldsymbol{\alpha}\cdot\nabla\widetilde{\chi}\,R_{\mathbf{A}}(iy)\,i\boldsymbol{\alpha}\cdot\nabla\chi\,R_{\mathbf{A}}(iy)\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\Big\rangle\Big|\frac{dy}{2\pi} \\
&\quad= \int_{\mathbb{R}} \Big|\Big\langle\, \zeta\,D_{\mathbf{A}}\,\varphi \,\Big|\, R_{\mathbf{A}}(iy)\,\Upsilon_{0,1/2}(iy)\,i\boldsymbol{\alpha}\cdot\nabla\widetilde{\chi}\,R_{\mathbf{A}}(iy)\,\Upsilon_{0,1/2}(iy)\,\times \\
&\qquad\qquad\qquad \times\, i\boldsymbol{\alpha}\cdot\nabla\chi\,R_{\mathbf{A}}(iy)\,\Upsilon_{0,1/2}(iy)\,\psi\,\Big\rangle\Big|\frac{dy}{2\pi}\,.
\end{aligned}$$

In the last step we repeatedly applied (3.16). Commuting ζ and $D_{\mathbf{A}}$ and using $\|D_{\mathbf{A}}\,R_{\mathbf{A}}(iy)\| \leqslant 1$, $\|R_{\mathbf{A}}(iy)\|^2 \leqslant (1+y^2)^{-1}$, and the fact that $\|\Upsilon_{0,1/2}(iy)\|$ is uniformly bounded in $y \in \mathbb{R}$, we readily deduce that

$$\big|\big\langle\, D_{\mathbf{A}}\,\varphi \,\big|\, H_{\mathrm{f}}^{1/2}\,\zeta\,P_{\mathbf{A}}^{+}\,\chi\,\check{H}_{\mathrm{f}}^{-1/2}\,\psi\,\big\rangle\big| \,\leqslant\, C(\zeta,\chi,\widetilde{\chi},d_1,d_4)\,\|\varphi\|\,\|\psi\|\,,$$

which implies (A.10). The bound (A.11) follows from (A.10) and the inequality

$$\|\,|\mathbf{x}|^{-1}\,\varphi\,\|^2 \,\leqslant\, 4\,\|\,D_{\mathbf{A}}\,\varphi\,\|^2 + 4\,\|\check{H}_{\mathrm{f}}^{1/2}\,\varphi\|\,, \qquad \varphi \in \mathcal{D}(D_{\mathbf{0}} \otimes H_{\mathrm{f}}^{1/2})\,,$$

which is a simple consequence of standard arguments (see, e.g., [10, Equation (4.7)]). □

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Laplace Transform Representations and Paley–Wiener Theorems for Functions on Vertical Strips

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Abstract. We consider the problem of representing an analytic function on a vertical strip by a bilateral Laplace transform. We give a Paley–Wiener theorem for weighted Bergman spaces on the existence of such representations, with applications. We generalise a result of Batty and Blake, on abscissae of convergence and boundedness of analytic functions on halfplanes, and also consider harmonic functions. We consider analytic continuations of Laplace transforms, and uniqueness questions: if an analytic function is the Laplace transform of functions f_1, f_2 on two disjoint vertical strips, and extends analytically between the strips, when is $f_1 = f_2$? We show that this is related to the uniqueness of the Cauchy problem for the heat equation with complex space variable, and give some applications, including a new proof of a Maximum Principle for harmonic functions.

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1 Introduction and notation

We are concerned with Laplace transforms: for an analytic function F on $\{a < \mathrm{Re}(z) < b\}$, we would like to know when

$$F(z) = \mathcal{L}h(z) \sim \int_{t=-\infty}^{\infty} e^{-zt} h(t)\, dt \sim \int_{t=-\infty}^{\infty} e^{-xt} h(t) e^{-iyt}\, dt$$

for some h, in some sense: either as an absolutely convergent Lebesgue integral, or as the L^2 or tempered distribution Fourier transform of $e^{-xt}h(t)$. Our normalisation of the Fourier transform is

$$\widehat{f}(\omega) \sim \int_{t=-\infty}^{\infty} e^{-i\omega t} f(t)\, dt, \qquad f(t) \sim \frac{1}{2\pi} \widehat{\widehat{f}}(-t).$$

In Section 2 we give a fairly general Paley–Wiener theorem which guarantees the existence of such an h for analytic functions F in certain weighted Bergman spaces, with applications. In Section 3 we generalise a result of C. Batty and M. D. Blake concerning bounded functions on halfplanes; we obtain the same result, but under weaker assumptions, as well as a similar result for harmonic functions.

In Section 4 we consider the *uniqueness* problem, which is important because analytic functions can sometimes be represented by Laplace transforms of different h on disjoint vertical strips. We obtain an explicit formula for analytic continuation under quite mild conditions, and relate this to the heat equation. Thus uniqueness theorems on the heat equation immediately give uniqueness theorems for boundary values of harmonic functions; see Corollaries 4.5, 4.6. Finally, Sections 5, 6 contain some longer proofs.

The problem of existence of Laplace transform representations for functions in certain spaces has been studied extensively; for example, see [4], [5], [9], [12], [20], [27], [29].

Given any domain $\Omega \subseteq \mathbb{C}$ and Banach space E, we write $\mathrm{Hol}(\Omega, E)$ for the set of all analytic functions $F : \Omega \to E$, or just $\mathrm{Hol}(\Omega)$ when $E = \mathbb{C}$. We need the theory of *Hardy spaces*: see [1], [10], [21], [25] and [26].

Let $\mathbb{C}_+ = \{z \in \mathbb{C} : \mathrm{Re}(z) > 0\}$ and $\mathbb{R}_+ = \{t \in \mathbb{R} : t \geqslant 0\}$. For any Banach space E, $1 \leqslant p < \infty$ and $F \in \mathrm{Hol}(\mathbb{C}_+, E)$, define

$$\|F\|_{H^p(\mathbb{C}_+,E)} = \sup_{r>0} \left(\int_{-\infty}^{\infty} \|F(r+iy)\|_E^p \frac{dy}{2\pi} \right)^{1/p}.$$

The set of all F with $\|F\| < \infty$ is the *Hardy space* $H^p(\mathbb{C}_+, E)$. When $E = \mathbb{C}$ we write simply $H^p(\mathbb{C}_+)$. We mainly use the case $p = 2$ with E a Hilbert space.

The classical Paley–Wiener Theorem says that $\mathcal{L} : L^2(\mathbb{R}_+, E) \to H^2(\mathbb{C}_+, E)$ is a *unitary operator* from L^2 *onto* H^2, *provided* that E is a Hilbert space:

$$\|f\|_{L^2(\mathbb{R}_+,E)} = \left(\int_{t=0}^{\infty} \|f(t)\|_E^2 \, dt \right)^{1/2} = \|\mathcal{L}f\|_{H^2(\mathbb{C}_+,E)},$$

and $\mathcal{L}^{-1} : H^2(\mathbb{C}_+, E) \to L^2(\mathbb{R}_+, E)$ is well–defined. Here, we are thinking of $H^2(\mathbb{C}_+, E) \subset L^2(i\mathbb{R}, E)$ in terms of a.e. boundary values.

2 Hilbert space Paley–Wiener type results

THEOREM 2.1 *Let* $-\infty \leqslant a < b \leqslant +\infty$, *let* E *be a Hilbert space, and let* $\Omega = \{z \in \mathbb{C} : a < \mathrm{Re}(z) < b\}$.

Suppose that $v : (a,b) \to [0, +\infty]$ *is Lebesgue measurable, with* $v > 0$ *almost everywhere. For any* $F \in \mathrm{Hol}(\Omega, E)$, *define*

$$\|F\|^2_{L^2(\Omega,v,E)} = \frac{1}{2\pi} \int_{x=a}^{b} \int_{y=-\infty}^{\infty} \|F(x+iy)\|_E^2 \, v(x) \, dy \, dx.$$

For any $h : \mathbb{R} \to E$ *strongly measurable, define*

$$N_v(h)^2 = \int_{t\in\mathbb{R}} \|h(t)\|_E^2 \left(\int_{x=a}^{b} e^{-2xt} v(x)\, dx \right) dt.$$

Then, *whenever* $N_v(h) < \infty$, *we have* $N_v(h) = \|\mathcal{L}h\|_{L^2(\Omega,v,E)}$.
Conversely, *let* $F \in \mathrm{Hol}(\Omega, E)$ *with* $\|F\|_{L^2(\Omega,v,E)} < \infty$. Assume also *that:*

$$\forall\, a < \alpha < \beta < b, \quad \exists\, \varepsilon(\alpha,\beta) > 0 \text{ such that } \int_{\alpha}^{\beta} v(x)^{-\varepsilon(\alpha,\beta)} dx < \infty. \tag{1}$$

Then: $\exists\, h$ *such that* $F = \mathcal{L}h$ *on* Ω, *and* $N_v(h) = \|F\|_{L^2(\Omega,v,E)}$. *Furthermore,* $F \in L^2(c + i\mathbb{R})$ *for* every $a < c < b$, *so* h *is given by the standard Bromwich Inversion Formula*

$$h(t) \sim \frac{1}{2\pi} \int_{y=-\infty}^{\infty} F(c+iy) e^{ct} e^{iyt}\, dy \sim \frac{1}{2\pi i} \int_{c+i\mathbb{R}} F(z) e^{zt}\, dz,$$

in the sense of $L^2(\mathbb{R}, E)$ *Fourier transforms.*

The paper [11] proves this result in the special case $a = 0$, $b = \infty$ and $v(x) = x^r$ with $r \geqslant 0$, and gives some applications. However, their method is different and probably cannot be generalised (*the conformal transformation* $\frac{1-z}{1+z}$ *induces an isometric isomorphism with a weighted Bergman space on the disc, for which* $(z^n)_{n\geqslant 0}$ *is an orthogonal basis*). Other related results and examples are given in Section 2 of [19].

Proof: The proof that $N_v(h) < \infty$ implies $\mathcal{L}h \in L^2(\Omega, v, E)$ with the same norm is not hard: by Fubini's Theorem, $\int_{x=a}^{b} \|e^{-xt}h(t)\|_{L^2(\mathbb{R},E)}^2 v(x)\, dx < \infty$. Thus $e^{-xt}h(t) \in L^2$ for a.e. $x \in (a, b)$, because $v > 0$ a.e. Now the Plancherel Theorem can be applied to the function $e^{-xt}h$, for a.e. x, and integrating with $v(x)dx$ gives the result.

For the converse: first, let $a < \alpha < \beta < b$. We must show that F is *bounded* on $\{x + iy : \alpha \leqslant x \leqslant \beta\}$. Let $r > 0$ be sufficiently small, so that $a < \alpha - r < \alpha < \beta < \beta + r < b$. Fix $\varphi \in E^*$ and consider $F_\varphi(z) = \varphi(F(z))$. We have the following result, which is a substitute for the lack of subharmonicity of $|F_\varphi|^p$ when $p < 1$. See Lemma 2, p. 172 of [14], there attributed to Hardy and Littlewood; the proof is given also on p. 185 of [23]:

$$\forall\, p > 0, \qquad |F_\varphi(\lambda)| \leqslant C_p \left(\frac{1}{\pi r^2} \int_{|z-\lambda|<r} |F_\varphi(z)|^p\, dA(z) \right)^{1/p}, \tag{2}$$

with some $C_p < \infty$. (*This is true more generally for harmonic functions in several variables. The case* $p \geqslant 1$ *is trivial by the Mean Value Property*). By assumption, $\int_{\alpha-r}^{\beta+r} v(x)^{-\varepsilon} dx < \infty$ for some $\varepsilon > 0$. Now let $p = 2\varepsilon(1+\varepsilon)^{-1}$. Apply Hölder's inequality with exponent $2/p$ to obtain that

$$\int_{|z-\lambda|<r} \|F(z)\|^p\, dA(z) = \int_{|z-\lambda|<r} \|F(z)\|^p v(x)^{p/2} v(x)^{-p/2}\, dA(z)$$

is bounded by a multiple of $\left(\int_{|z-\lambda|<r} \|F(z)\|^2 v(x)\, dA(z)\right)^{p/2}$, independently of λ with $\alpha \leqslant \mathrm{Re}(\lambda) \leqslant \beta$. By (2) and (1), we now have $|F_\varphi(\lambda)| \leqslant K\|\varphi\|_{E^*}$, so indeed F is bounded on $\{\alpha \leqslant x \leqslant \beta\}$ as required.

Second, suppose that $\int_{-\infty}^{\infty} \|F(x+iy)\|^2\, dy < \infty$ for $x = \alpha, \beta$, where $a < \alpha < \beta < b$. Thus for each $Y > 0$, Cauchy's Integral Formula gives

$$F(\lambda) = \frac{1}{2\pi i}\int_{\partial R_Y} \frac{F(z)}{z-\lambda} dz \quad \text{for all } \lambda \in R_Y = (\alpha,\beta)\times(-Y,Y).$$

But F is bounded on R_Y, uniformly in Y, by above; so we can let $Y \to \infty$ for each fixed λ to obtain

$$F(\lambda) = \frac{1}{2\pi i}\left(\int_{\beta+i\mathbb{R}} - \int_{\alpha+i\mathbb{R}}\right) \frac{F(z)}{z-\lambda} dz, \quad \text{whenever } \mathrm{Re}(\lambda) \in (\alpha,\beta).$$

Now $\int_{\alpha+i\mathbb{R}} \frac{F(z)}{z-(\alpha+\omega)} dz$, as a function of $\omega \in \mathbb{C}_+$, is the Szegö projection of the $L^2(i\mathbb{R}, E)$ function $F(iy+\alpha)$ onto the Hardy space $H^2(\mathbb{C}_+, E)$, and so by the Paley–Wiener Theorem it can be represented as $\mathcal{L}f_1$ for some $f_1 \in L^2(\mathbb{R}_+, E)$. We can consider similarly $\int_{\beta+i\mathbb{R}} \frac{F(z)}{z-(\beta-\omega)} dz$. Thus

$$F(\lambda) = -\int_{t=0}^{\infty} e^{-(\lambda-\alpha)t} f_1(t)\, dt + \int_{t=0}^{\infty} e^{-(\beta-\lambda)t} f_2(t)\, dt,$$

and so $F(\lambda) = \mathcal{L}h(\lambda) = \int_{t=-\infty}^{\infty} e^{-\lambda t} h(t)\, dt$ on $\{\alpha < \mathrm{Re}(\lambda) < \beta\}$, with

$$\int_0^{\infty} \|e^{-\alpha t} h(t)\|^2\, dt, \int_0^{\infty} \|e^{\beta t} h(-t)\|^2\, dt < \infty.$$

This shows that $e^{-ct}h(t) \in L^2(\mathbb{R}, E)$ for each $\alpha < c < \beta$.

Now $v > 0$ a.e., so $\int_{-\infty}^{\infty} \|F(x+iy)\|^2\, dy < \infty$ for a.e. $x \in (a,b)$. So choose sequences $(\alpha_j) \searrow a$ and $(\beta_j) \nearrow b$ such that this holds with $x = \alpha_j, \beta_j$. Then $F = \mathcal{L}h_j$ on $\{\alpha_j < \mathrm{Re}(\lambda) < \beta_j\}$ for each j. By uniqueness of the Fourier transform we must have $h_j \equiv h_1 = h$ a.e.

So finally $F = \mathcal{L}h$ on $\{a < \mathrm{Re}(\lambda) < b\}$, and Plancherel's Theorem gives

$$\frac{1}{2\pi}\int_{y=-\infty}^{\infty} \|F(x+iy)\|^2 dy = \int_{t=-\infty}^{\infty} e^{-2xt}\|h(t)\|^2\, dt$$

for each $a < x < b$. Hence $N_v(h) = \|F\|_{L^2(\Omega,v,E)}$.

□

Similarly, with the Hausdorff–Young theorem and Paley–Wiener theorem for H^p, we can easily obtain the following result:

Theorem 2.2 *Let $F \in \mathrm{Hol}\{a < \mathrm{Re}(z) < b\}$, let $1 < p \leqslant 2$, let v satisfy the same conditions as Theorem 2.1, and suppose that*

$$\int_{x=a}^{b}\int_{y=-\infty}^{\infty} |F(x+iy)|^p\, v(x)\, dy\, dx < \infty. \tag{3}$$

Then there exists some h *such that* $F = \mathcal{L}h$ *and*

$$\int_{x=a}^{b} \left(\int_{t=-\infty}^{\infty} e^{-p'xt} |h(t)|^{p'} \, dt \right)^{p-1} v(x) \, dx < \infty. \tag{4}$$

We can consider Dirichlet–type norms also; for example:

Corollary 2.3 *Let* $F \in \mathrm{Hol}(\mathbb{C}_+, E)$*, for a Hilbert space* E*. Then*

$$\iint_{\mathbb{C}_+} \|F'(z)\|^2 x \, dx \, dy < \infty \qquad \Longleftrightarrow \qquad F \in H^2(\mathbb{C}_+, E) + \{\textit{constants}\}.$$

This is obvious, since $\int_0^\infty \|h(t)\|^2 dt/t^2 < \infty$ if and only if $h(t)/t \in L^2(\mathbb{R}_+, E)$ if and only if $\mathcal{L}(h(t)/t) \in H^2$.

Corollary 2.4 *Let* $F \in \mathrm{Hol}\{0 < \mathrm{Re}(z) < R\}$ *be bounded, for some* $0 < R \leqslant +\infty$*. Then* $\exists\, g : \mathbb{R} \to \mathbb{C}$ *such that* $F(z) = z\mathcal{L}g(z)$*, and*

$$\int_{-\infty}^{0} e^{2R|t|} |g(t)|^2 \, dt < \infty, \qquad \sup_{T > 1/R} \left(\frac{1}{T} \int_0^T |g(t)|^2 \, dt \right) < \infty.$$

Also $\sup_{0 \leqslant c \leqslant R} \|e^{-ct} g\|_{BMO(\mathbb{R})} < \infty$*. In particular,*

$$\int_{t=0}^{\infty} \frac{|g(t)| + e^{-Rt}|g(-t)|}{1+t^2} dt < \infty.$$

In the case $R = +\infty$*, we have* $g(t) = 0$ *for all* $t < 0$*.*

$BMO(\mathbb{R})$ is the very important Bounded Mean Oscillation space, discussed in [1], [16], [23] and many other books, which often serves as a useful substitute for $L^\infty(\mathbb{R})$. For locally integrable $f : \mathbb{R} \to \mathbb{C}$ we have

$$\|f\|_{BMO(\mathbb{R})} = \sup_I |f - f_I|_I, \quad \text{where} \quad f_I = \frac{1}{|I|} \int_I f(t) \, dt,$$

I ranges over all *bounded intervals* of $\mathbb{R}$, and $|I|$ is the *length*.

Proof: The existence of g is immediate from Theorem 2.1, if we consider $G(z) = F(z)/z$ and take, e.g. $v(x) = x/(1+x^3)$. The estimates follow from Plancherel's Theorem:

$$\int_{-\infty}^{\infty} e^{-2xt} |g(t)|^2 \, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left| \frac{F(x+iy)}{x+iy} \right|^2 dy \ll \frac{1}{x}.$$

For the estimate with $t > 0$, let $T > 1/R$ and consider $\int_{t=0}^{T}$ only with $x = 1/T$. For $\int_{t=-\infty}^{0}$ we just let $x \nearrow R$.

For the BMO result, let $0 < c < R$. Then $\frac{F(c+iy)}{c+iy}$ is an L^2 function of $y \in \mathbb{R}$, with $\left|\frac{F(c+iy)}{c+iy}\right| \leqslant \frac{\sup|F|}{|y|}$. We have

$$e^{-ct}g(t) \sim \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{F(c+iy)}{c+iy} e^{iyt}\, dy.$$

Now apply Lemma 2.5 below to get $\|e^{-ct}g\|_{BMO(\mathbb{R})} \leqslant K$ for some K independent of c. For $c = 0$ and $c = R$, choose sequences $c_j \searrow 0$ and $c_j \nearrow R$ and use Dominated Convergence: for each interval I, $(e^{-c_j t}g)_I \to g_I$ or $(e^{-Rt}g)_I$ as appropriate. Then $|e^{-c_j t}g - (e^{-c_j t}g)_I|_I$ also converges appropriately; since the BMO norm is given by a supremum over all I, we have the result.
□

Lemma 2.5 *If* $f \in L^2(\mathbb{R})$ *then* $\left\|\hat{f}\right\|_{BMO(\mathbb{R})} \leqslant C\sup_{\beta\in\mathbb{R}}|\beta f(\beta)|$, *where* C *is a universal constant independent of* f.

Proof: By considering the restrictions of f to $\mathbb{R}_+$ and $\mathbb{R}_-$ separately, it is enough to consider $f \in L^2(\mathbb{R}_+)$ with $|\beta f(\beta)| \leqslant 1$. Take $u \in L^2(\mathbb{R}_+)$ and consider the convolution $(k * u)(\alpha) = \int_{s=0}^{\alpha} k(\alpha - s)u(s)\, ds$. By Hardy's Inequality (see [18]),

$$\int_{\alpha=0}^{\infty} |(\beta f * u)(\alpha)|^2 \frac{d\alpha}{\alpha^2} \leqslant \int_{\alpha=0}^{\infty}\left(\frac{1}{\alpha}\int_{s=0}^{\alpha}|u(s)|\, ds\right)^2 d\alpha$$
$$\leqslant 4\int_{s=0}^{\infty}|u(s)|^2 ds.$$

Taking Laplace transforms and using (the easy half of) Theorem 2.1 gives

$$\iint_{\mathbb{C}_+} |\mathcal{L}(\beta f)(z)\mathcal{L}u(z)|^2 x\, dx\, dy \leqslant K\|\mathcal{L}u\|^2_{H^2(\mathbb{C}_+)}.$$

But this says exactly that $|\mathcal{L}(\beta f)(z)|^2 x\, dx\, dy = |(\mathcal{L}f)'(z)|^2 x\, dx\, dy$ is a *Carleson Measure* on $\mathbb{C}_+$. Hence $\mathcal{L}f \in \mathrm{Hol}(\mathbb{C}_+)$ is the *Poisson integral* of some function $U \in BMO$, by [13]. But also $\mathcal{L}f \in H^2(\mathbb{C}_+)$, and so $\mathcal{L}f$ is the Poisson integral of its boundary function $\hat{f}$. Hence $\hat{f} = U \in BMO$ as required.
□

In Theorem 3.1 below we obtain further results on g, assuming extra conditions on F (*decay behaviour on a vertical line*).

3 Results assuming decay on a vertical line

The following theorem generalises the main result of [3].

Theorem 3.1 *Let* $0 < R \leqslant +\infty$ *and* $\Omega = \{z : 0 < \mathrm{Re}(z) < R\}$. *Let* E *be a Banach space, and let* $F \in \mathrm{Hol}(\Omega, E)$ *be bounded. Assume that* $\exists\, 0 < c < R$, $0 < \delta \leqslant 1$ *and* $\nu > 1$ *such that*

$$\forall\, \varphi \in E^*, \qquad \int_{y=-\infty}^{\infty} \frac{\left|\varphi(F(c+iy))\right|^{\nu}}{(1+|y|)^{1-\delta}} dy < \infty. \tag{5}$$

Then *there exists some continuous* $g : \mathbb{R} \to E$ *with* $F(z) = z\mathcal{L}g(z)$ *for all* $z \in \Omega$, *such that*

$$\|g(t)\| \leqslant \begin{cases} M(1+t) & \textit{for } t > 0, \\ Me^{Rt}(1+|t|) & \textit{for } t < 0. \end{cases} \tag{6}$$

In the case $R = +\infty$, *we have* $g(t) = 0$ *for all* $t \leqslant 0$. *Also* g *satisfies local Hölder estimates: there is some* $M < \infty$ *such that*

$$\|g(t+s) - g(s)\| \leqslant Me^{cs}t^{\delta/\nu} \qquad (\forall\, s \in \mathbb{R},\ 0 < t < 1). \tag{7}$$

The proof is given in Section 5. Of course we can get additional information about $|\varphi(g(t))|^2$ by applying Corollary 2.4 above to $\varphi \circ F$.
In [3] the main result was the estimate (6) for the case $R = +\infty$ only, assuming the much stronger condition

$$F = \mathcal{L}f \quad \text{with} \quad \int_0^\infty \|e^{-rt}f(t)\|^p dt < \infty, \quad p > 1, r > 0. \tag{8}$$

[3] also explains that (8) is not sufficient in the case $p = 1$. Under assumption (8), we would have $g(t) = \int_0^t f(s)\,ds$. By increasing r if necessary and using Hölder's inequality, we could take $1 < p \leqslant 2$ without loss of generality. Then the Hausdorff–Young Theorem would give (5) for $c = r$ with $\nu = (1 - 1/p)^{-1} = p' \geqslant 2$ and $\delta = 1$. The estimate (6) is best possible in general, even under the extra assumption (8), as shown in [2].
Additionally (7), which is a *conclusion* of our theorem, would follow automatically from the assumption (8).
In the case $R = +\infty$, we have a similar result for *harmonic* functions:

THEOREM 3.2 *Let* $F : \mathbb{C}_+ \to E$ *be a bounded* harmonic *function, where* E *is a Banach space. Assume that* (5) *holds with* $c > 0$.
Then: *there exist* $g_j : \mathbb{R}_+ \to E$ *continuous,* $j = 1, 2$, *such that*

$$g_j(0) = 0, \quad \|g_j(t)\| \leqslant K(1+t^2),$$
$$F(z) = z\,\mathcal{L}g_1(z) + \bar{z}\mathcal{L}g_2(\bar{z}) \textit{ on } \mathbb{C}_+,$$

and g_1, g_2 *satisfy the same Hölder estimate* (7) *from Theorem 3.1.*

See Section 6 for the proof. Unfortunately, the case $R < \infty$ is unsatisfactory. For example, there is no function g such that $z + a = z\mathcal{L}g(z)$, with $a \in \mathbb{C}$ constant. Thus $2\mathrm{Re}(z) = z + \bar{z}$ is harmonic and bounded on $\{0 < \mathrm{Re}(z) < 1\}$ but *cannot* be written as $z\mathcal{L}g_1(z) + \bar{z}\mathcal{L}g_2(\bar{z})$ for any functions g_1, g_2.

4 UNIQUENESS CONDITIONS

It is natural to consider *uniqueness*: if $\mathcal{L}f_1 = \mathcal{L}f_2$ on $\{a < \mathrm{Re}(z) < b\}$, in any reasonable sense, then $f_1 = f_2$ by uniqueness of Fourier transforms. However, this does not answer the following:

QUESTION 4.1 *Let $a_1 < b_1 < a_2 < b_2$ and $F \in \mathrm{Hol}\{a_1 < \mathrm{Re}(z) < b_2\}$, with*

$$\sup_{a_j<c<b_j} \int_{-\infty}^{\infty} |F(c+iy)|^2\,dy < \infty, \quad \textit{for } j = 1,2,$$

so that $F = \mathcal{L}f_j$ on $\{a_j < \mathrm{Re}(z) < b_j\}$ for some (uniquely determined) f_1, f_2, by Theorem 2.1. When do we have $f_1 = f_2$?

In contrast to Laurent series on concentric annuli $\{r_j < |z| < R_j\}$, it is possible to have $f_1 \neq f_2$. The paper [24] considers

$$G \in \mathrm{Hol}(\mathbb{C}), \qquad G(z) = \int_{t=0}^{\infty} e^{zt} t^{-t} dt.$$

Then G is entire, and bounded on $\{|\mathrm{Im}(z)| > \pi/2 + \delta\}$ for each $\delta > 0$. Define $F(z) = -iG(iz)$. By Cauchy's Theorem as in [24] we obtain

$$F(z) = \int_{s=0}^{\infty} e^{-zs} \exp\left(-is\log s + \frac{\pi s}{2}\right) ds, \qquad \mathrm{Re}(z) > \frac{\pi}{2}.$$

Since $G(\bar{z}) = \overline{G(z)}$, we have $F(-\bar{z}) = -\overline{F(z)}$. Thus

$$F(z) = -\int_{s=-\infty}^{0} e^{-zs} \exp\left(-is\log(-s) - \frac{\pi s}{2}\right) ds, \qquad \mathrm{Re}(z) < -\frac{\pi}{2}.$$

So F is entire and represented by *different* bilateral Laplace transforms on $\{x > \pi/2\}$, $\{x < -\pi/2\}$, even though (*using Plancherel's Theorem*)

$$\int_{-\infty}^{\infty} |F(x+iy)|^2\,dy \leqslant M\left(|x| - \frac{\pi}{2}\right)^{-1} \quad \text{whenever } |x| > \pi/2.$$

Thus by rescaling, for any $\epsilon > 0$ the "gap" $\{|x| < \epsilon\}$ is "unsafe": crossing the gap can change the Laplace transform function. However, we shall prove below that the gap $\{x = 0\}$ can be safely crossed under quite mild restrictions. First we derive an *explicit formula* for analytic continuation of Laplace transforms.

THEOREM 4.2 *Let $\Omega = \{z : a < \mathrm{Re}(z) < b\}$ and $F \in \mathrm{Hol}(\Omega, E)$, with E a Banach space. Assume that $a < c < b$, $\kappa > 0$, and*

$$\int_{-\infty}^{\infty} \|F(c+iy)\| \exp(-\kappa y^2)\,dy < \infty. \tag{9}$$

Define $F_\sigma \in \mathrm{Hol}(\mathbb{C}, E)$, for sufficiently small $\sigma > 0$, by

$$\begin{aligned} F_\sigma(z) = F_{\sigma,c}(z) &= \int_{\lambda\in c+i\mathbb{R}} F(\lambda) \exp\left(\frac{(\lambda - z)^2}{2\sigma^2}\right) \frac{d\lambda}{i\sigma\sqrt{2\pi}} \\ &= \int_{y=-\infty}^{\infty} F(c+iy) \exp\left(\frac{(c+iy-z)^2}{2\sigma^2}\right) \frac{dy}{\sigma\sqrt{2\pi}}. \end{aligned}$$

Then $\sup_C |F_\sigma - F| \leqslant K(C)\sigma^2$ for each fixed compact $C \subset \Omega$. In particular, $F_\sigma \to F$ locally uniformly on Ω, as $\sigma \to 0^+$.

Proof: Define $G(\lambda, z) = \frac{F(\lambda)}{i\sigma\sqrt{2\pi}} \exp\left(\frac{(\lambda-z)^2}{2\sigma^2}\right)$, so that

$$\|G(\lambda, x+iy)\| = \frac{\|F(\lambda)\|}{\sigma\sqrt{2\pi}} \exp\left(\frac{|x-\mathrm{Re}(\lambda)|^2 - |y-\mathrm{Im}(\lambda)|^2}{2\sigma^2}\right).$$

For each fixed $z \in \mathbb{C}$, $F_\sigma(z)$ is the integral of $G(\lambda, z)$ over the contour $c + i\mathbb{R}$, which converges for $1/2\sigma^2 > \kappa$ by condition (9). Since $G(\lambda, z)$ is an analytic function of λ, we can use Cauchy's Theorem with the same contour as in Theorem 3.1. Pick $\omega = \omega_1 + i\omega_2 \in \Omega$ and fix a square $\Sigma = \{|x-\omega_1|, |y-\omega_2| \leqslant \delta\} \subset \Omega$. Let Y be large, much larger than δ, and consider the contours

$$\begin{aligned} \Gamma(x) &= \{\mathrm{Re}(\lambda) = x, & |\mathrm{Im}(\lambda) - \omega_2| \leqslant Y\},\\ \Gamma_Y^{\pm}(x) &= \{\mathrm{Re}(\lambda) \in [x, c], & \mathrm{Im}(\lambda) = \omega_2 \pm Y\},\\ \Gamma' &= \{\mathrm{Re}(\lambda) = c, & |\mathrm{Im}(\lambda) - \omega_2| \geqslant Y\}. \end{aligned}$$

For $\lambda \in \Gamma_Y^{\pm}(x)$, we have

$$\|G(\lambda, z)\| \leqslant \sup_{\mu \in I} \|F(\mu)\| \cdot \sigma^{-1} \exp\left(\frac{M - Y^2/2}{2\sigma^2}\right),$$

uniformly for $z \in \Sigma$, where $I = \Gamma_Y^{\pm}(\omega_1 - \delta)$ or $I = \Gamma_Y^{\pm}(\omega_1 + \delta)$ as appropriate (*depending on whether* $\omega_1 < c$ *or* $\omega_1 > c$). We are using $(Y-y)^2 > Y^2/2$ and $(c-x)^2 < M$.

Thus $\int_{\Gamma_Y^{\pm}(x)} G\, d\lambda \to 0$ rapidly as $\sigma \to 0$, uniformly in z, as long as Y is large enough. By condition (9) again, also $\int_{\Gamma'} G\, d\lambda \to 0$ rapidly as $\sigma \to 0$, uniformly for $z \in \Sigma$. Finally, the integral over $\Gamma(x)$ is a standard Gaussian convolution approximation to $F(z)$:

$$\int_{\Gamma(x)} G(\lambda, x+iy)\, d\lambda = \int_{\omega_2 - Y}^{\omega_2 + Y} F(x+iu) \exp\left(\frac{-(y-u)^2}{2\sigma^2}\right) \frac{du}{\sigma\sqrt{2\pi}}.$$

After Y is chosen, $F(t+iu)$ is then bounded on the tall, narrow rectangle $|t-\omega_1| \leqslant \delta$, $|u-\omega_2| \leqslant Y$. If we approximate $F(x+iu)$ by its Taylor series about $x+iy$, it is now routine to verify that $\int_{\Gamma(x)} G(\lambda, x+iy)\, d\lambda = F(x+iy) + O(\sigma^2)$, *uniformly* for $|x-\omega_1|, |y-\omega_2| < \delta/2$, say. The errors from the other contours are much smaller, being $O(\exp(-\nu/\sigma^2))$ for some $\nu > 0$.
□

Corollary 4.3 *With F as in Theorem 4.2 and $E = \mathbb{C}$, suppose that*

$$\exists\, 1 \leqslant p \leqslant 2 \quad \textit{such that} \quad \int_{-\infty}^{\infty} |F(c+iy)|^p\, dy < \infty.$$

Then

$$F(z) = \lim_{\sigma \to 0^+} \int_{t=-\infty}^{\infty} e^{-zt} h(t) \exp(-\sigma^2 t^2/2)\, dt \tag{10}$$

locally uniformly for $z \in \Omega$*, for some measurable* h *satisfying*

$$\int_{-\infty}^{\infty} |h(t)| e^{-\delta t^2}\, dt < \infty \quad \forall \delta > 0.$$

Proof: We use the Hausdorff–Young Theorem. Set

$$h(t)e^{-ct} \sim \frac{1}{2\pi} \widehat{F(c+iy)}(-t) \in L^{p'}(\mathbb{R}),$$

for $p' = (1 - 1/p)^{-1}$ the conjugate exponent to p. This is well–defined for a.e. $t \in \mathbb{R}$. Now $\int \widehat{h(t)e^{-ct}}(y) g(y)\, dy = \int h(t)e^{-ct} \widehat{g}(t)\, dt$ for every Schwartz function g. Now put $F(c+iy) \sim \widehat{he^{-ct}}(y)$ in the definition of $F_{\sigma,c}(z)$ and calculate.
□

Notice that (10) is just a weak kind of Laplace transform representation for F. It says that a particular Abelian summability method assigns the value $F(z)$ to the formal integral "$\int_{-\infty}^{\infty} e^{-zt} h(t)\, dt$", even though this integral may diverge. See [17] for much more on these topics; unfortunately the classical results given there appear to be inadequate for our problem.

Corollary 4.4 *Let* $\Omega = \{z : a < \mathrm{Re}(z) < b\}$ *and* $F \in \mathrm{Hol}(\Omega)$*. Suppose that there exist* $a < c_1 < c_2 < b$ *and* f_1, f_2 *such that*

$$F(c_j + iy) \sim \int_{t=-\infty}^{\infty} f_j(t) e^{-c_j t} \exp(-iyt)\, dt \qquad (y \in \mathbb{R}, \quad j = 1, 2),$$

as Fourier transforms of $f_j(t)e^{-c_j t} \in L^2(\mathbb{R})$*. Define*

$$H(z,v) = \int_{t=-\infty}^{\infty} \big(f_1(t) - f_2(t) \big) \exp(izt - vt^2) dt$$

for $z \in \mathbb{C}$*,* $v > 0$*. Then* H *has a continuous extension* $H : i\Omega \times [0,\infty) \to \mathbb{C}$ *satisfying*

$$\frac{\partial^2 H}{\partial z^2} = \frac{\partial H}{\partial v}, \qquad H(z,0) \equiv 0 \quad (z \in i\Omega).$$

Proof: By Corollary 4.3, equation (10) holds for both $h = f_1$ and $h = f_2$. Therefore, $H(z,v) \to F(-iz) - F(-iz) = 0$ as $v \to 0^+$, for each $z \in i\Omega$. Because this convergence is locally uniform, we have the required continuity of H. Finally, the complex heat equation $\frac{\partial^2 H}{\partial z^2} = \frac{\partial H}{\partial v}$ follows immediately by differentiating under the integral sign.
□

The letter t is normally used for the time variable, but we use $v = \sigma^2/2$ (for *variance*, with an extra factor of 2). Now we can apply known results on the heat equation. The papers [6], [30] prove many results about functions on discs. The following corollaries are closely related (after applying a conformal transformation), but our proofs are easier and quite different.

Corollary 4.5 *Let* $F \in \mathrm{Hol}(\{-1 < x < 1\})$ *and* $A, B, r > 0$*, with*

$$\int_{-\infty}^{\infty} |F(x+iy)|^2 dy \leqslant A \exp(B|x|^{-r}), \quad \forall\, x \neq 0.$$

Then $\sup_{-1<x<1} \int_{-\infty}^{\infty} |F(x+iy)|^2 dy < \infty$*. In particular,* F *is bounded on* $|x| < 1 - \epsilon$*, for each* $\epsilon > 0$*.*

Notice that, a priori, it is not obvious that any estimate for $|F(iy)|$ is possible: $\exp(B|x|^{-r})$ grows so rapidly as $|x| \to 0$ that any simple attempt based on the Mean Value Property must fail.

Proof: First, by Theorem 3.1, we know that $F = \mathcal{L}f_+$ on $\{0 < x < 1\}$ and $F = \mathcal{L}f_-$ on $\{-1 < x < 0\}$, with $\int_{-\infty}^{\infty} e^{-2\delta t}|f_+(t)|^2\, dt \ll \exp(B\delta^{-r})$, and similarly for f_-. Now consider $\varphi = f_+ - f_-$. Then

$$\int_{-\infty}^{\infty} e^{-2\delta|t|}|\varphi(t)|^2\, dt \ll \exp(B\delta^{-r}).$$

Following Corollary 4.4, define

$$H(y,v) = \int_{-\infty}^{\infty} \exp(iyt - vt^2)\varphi(t)\, dt$$

for $y \in \mathbb{R}$ and $v > 0$. Then H satisfies the heat equation and extends to be continuous on $\{v \geqslant 0\}$, with $H(y,0) \equiv 0$. We calculate

$$\begin{aligned} |H(y,v)| &\leqslant \left(\int_{-\infty}^{\infty} e^{-\delta|t|}|\varphi(t)|\, dt\right) \sup_{\tau\in\mathbb{R}} \exp(\delta|\tau| - v\tau^2) \\ &\ll \delta^{-1/2}\exp(B\delta^{-r}/2)\exp(\delta^2/4v) \leqslant \exp\left(C\delta^{-r} + \frac{\delta^2}{4v}\right), \end{aligned}$$

for any $0 < \delta < 1$. We have used the Cauchy–Schwarz inequality and $\delta^{-1/2} < \exp(\delta^{-1/2}) \leqslant \exp(\delta^{-r})$, as long as $r \geqslant 1/2$, which we could clearly assume from the start. Notice that C does not depend on δ.

Now choose $\delta = v^\alpha$ with $\alpha = 1/(r+2)$, so that $\alpha r = 1 - 2\alpha$, to obtain

$$|H(y,v)| \leqslant A' \exp\left(\frac{C + 4^{-1}}{v^{1-2\alpha}}\right) = A'\exp(C'/v^\eta), \tag{11}$$

for all $y \in \mathbb{R}$, $0 < v < 1$, with $0 < \eta < 1$. Since $H = H(y,v)$ is a solution to the heat equation with $H(y,0) \equiv 0$, condition (11) implies that $H \equiv 0$. See [8], [15]. In general the condition $|H| \leqslant A(\epsilon)\exp(\epsilon/v)$ for each $\epsilon > 0$ is not sufficient, as shown in [7], but our proof works because we have an estimate for $A(\epsilon)$. Therefore $\varphi = 0$ and $f_+ = f_-$ almost everywhere, as required.

□

Corollary 4.6 *Let* $\Omega = \{x + iy : 0 < x < 1\}$. *Let* E *be a Banach space,* $F : \overline{\Omega} \to E$ *continuous, harmonic on* Ω*, and* $F \in L^\infty(\partial\Omega)$. *Suppose that* $A, B, r > 0$ *satisfy*

$$\|F(x+iy)\| \leqslant A\exp(B[x(1-x)]^{-r}) \qquad \forall\, 0 < x < 1, y \in \mathbb{R}.$$

Then $F \in L^\infty(\Omega)$ *with* $\sup_\Omega \|F\| = \sup_{\partial\Omega} \|F\|$.

This is a Maximum Principle, similar in some ways (*but quite different in other ways*) to the Phragmén–Lindelöf theorems.

Proof: By considering $\varphi \circ F$ for each $\varphi \in E^*$, it is enough to consider the case $E = \mathbb{C}$; by considering $\mathrm{Re}(F)$, $\mathrm{Im}(F)$, we can take $E = \mathbb{R}$. Now let $\widetilde{F}$ be the unique *bounded* harmonic function with $F = \widetilde{F}$ on $\partial\Omega$. For example, we could obtain $\widetilde{F}$ by conformal mapping and the well–known Poisson Formula for the disc. By considering $F - \widetilde{F}$, *we only need to prove the special case where* F *is real–valued, and zero on* $\partial\Omega$.

By the Schwarz Reflection Principle, we can extend F to be harmonic on $\mathbb{C}_+$ and continuous on $i\mathbb{R}$, by defining $F(n + x + iy) = -F(n - x + iy)$ repeatedly for $x \in [0, 1]$, $y \in \mathbb{R}$ and $n = 1, 2, 3, \ldots$.

Thus $|F| \ll \exp(C \cdot \mathrm{dist}(x, \mathbb{Z})^{-r})$, where dist means *distance*. We have $F = g + \bar{g}$ for some $g \in \mathrm{Hol}(\mathbb{C}_+)$. Now

$$g'(\lambda) = \frac{1}{2\pi r}\int_0^{2\pi} F(\lambda + re^{i\theta})e^{-i\theta}d\theta,$$

so that $|g'| \ll \exp(C'\mathrm{dist}(x, \mathbb{Z})^{-r})$, by simple estimates for F with the Mean Value Property. Also $\int_{n-1/2}^{n+1/2} |g'(t)|\, dt$ is independent of n, because of the reflection process used to extend F. Thus

$$\begin{aligned} |g(z)| &= \left| g(1) + \int_1^x g'(t)\, dt + i\int_0^y g'(x + is)\, ds \right| \\ &\leqslant A'(1 + |z|)\exp\left(\frac{C'}{\mathrm{dist}(x, \mathbb{Z})^r}\right). \end{aligned}$$

Now consider $h(z) = g(z)(1+z)^{-1}$. By applying Corollary 4.5 to h repeatedly on the domains $\{|x - n| < 1 - \epsilon\}$ (with trivial rescaling), we obtain $\int_{-\infty}^{\infty} |h(x + iy)|^2 dy \leqslant M(\epsilon)$ for all $x > \epsilon$, i.e. $h \in H^2(\{\mathrm{Re}(z) > \epsilon\})$ for each $\epsilon > 0$. Thus $h = \mathcal{L}u$ on $\mathbb{C}_+$ for some u on $\mathbb{R}_+$ with $\int_0^\infty e^{-\delta t}|u(t)|^2 dt < \infty$ for all $\delta > 0$. But now

$$0 = \frac{F(n)}{1+n} = 2\mathrm{Re}[h(n)] = \int_0^\infty e^{-nt}2(\mathrm{Re}\, u)(t)\, dt$$

for all $n = 1, 2, 3, \ldots$. So $\mathcal{L}(\mathrm{Re}\, u)$ is bounded and analytic on $\{\mathrm{Re}(z) > 1/2\}$, with a zero at each n, and thus identically zero everywhere by the Blaschke condition for zero sequences of Hardy space functions. Thus $\mathrm{Re}\, u = 0$ almost everywhere.

So $\bar{u} = -u$ a.e., and now $\overline{h(x)} = -h(x)$ for all $x > 0$, so that $F(x) = g(x) + \overline{g(x)} = 0$. Now the proof is finished; we have shown that $F = 0$ on $\{0 < x < 1\}$. Applying this to $F_\alpha = F(z + i\alpha)$ for each $\alpha \in \mathbb{R}$, we obtain that $F \equiv 0$, as required.
□
We remark, omitting the details, that Corollary 4.6 can be used to prove Corollary 4.5, so they are equivalent: given an analytic F on $\{|x| < 1\}$, consider $U(z) = F(z) - F(-\bar{z})$ on $\{0 \leqslant x \leqslant 1/2\}$.

5 proof of Theorem 3.1

We first prove (6). First consider the scalar case $E = \mathbb{C}$. By Theorem 2.1 applied to $F(z)/z$, we see immediately that $F(z)/z = \mathcal{L}g(z)$ for some g, given by

$$g(t) \sim \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{F(c+iy)}{c+iy} e^{(c+iy)t}\, dy \sim \frac{1}{2\pi i} \int_{c+i\mathbb{R}} \frac{F(z)}{z} e^{zt}\, dz.$$

If $R = +\infty$ then Theorem 2.1 also gives $g(t) \equiv 0$ for $t \leqslant 0$. But $\int_{c+i\mathbb{R}} \left|\frac{F(z)}{z}\right| |dz| < \infty$ by Hölder's inequality, so in fact $g : \mathbb{R} \to \mathbb{C}$ is *continuous* (after changing g on a set of measure zero).
The estimate $|g(t)| \leqslant M(1+t)$ for $t > 0$ was already proved in [3] for the special case $R = +\infty$ and $F \in L^q(c + i\mathbb{R})$ for some $q > 1$. But that proof needed only the estimate $\int_{|z|>\kappa} \frac{|F(z)|}{|z|} |dz| = O(\kappa^{-\epsilon})$ for some $0 < \epsilon < 1$, which follows from (5) by Hölder's inequality. The proof also applies without change when $R < \infty$. For $t < 0$, we can simply apply the result to $F(R - z)$.
The Hölder estimate (7) follows by direct calculation: we have

$$|g(t+s) - g(s)| \ll \int_{c+i\mathbb{R}} \left| \frac{F(z)}{z} \right| e^{cs} |e^{zt} - 1|\, |dz|.$$

By Hölder's inequality, this is

$$\ll e^{cs} \left(\int_{c+i\mathbb{R}} \frac{|F(z)|^\nu}{|z|^{1-\delta}} dy \right)^{1/\nu} \left(\int_{c+i\mathbb{R}} \frac{|e^{zt} - 1|^{\nu'}}{|z|^\alpha} |dz| \right)^{1/\nu'},$$

where $\alpha = \left(1 - \frac{1-\delta}{\nu}\right) \nu' = 1 + \delta \frac{\nu'}{\nu} > 1$. Since $|z| \approx c + |y| \approx 1 + |y|$, the second integral above is

$$\begin{aligned}
&\ll \int_{\mathbb{R}} \frac{|e^{(c+iy)it} - 1|^{\nu'}}{(1+|y|)^\alpha} dy \\
&\ll t^{\nu'} \int_{|c+iy|<t^{-1}} \frac{|c+iy|^{\nu'}}{(1+|y|)^\alpha} dy + \int_{|c+iy|>t^{-1}} \frac{dy}{(1+|y|)^\alpha} \\
&\ll t^{\nu'} \int_{|y|<At^{-1}} (1+|y|)^{\nu'-\alpha} dy + \int_{|y|>Bt^{-1}} \frac{dy}{(1+|y|)^\alpha} \\
&\ll t^{\nu'} (1/t)^{\nu'-\alpha+1} + (1/t)^{1-\alpha} \ll t^{\alpha-1}.
\end{aligned}$$

Here t is small, $A, B > 0$ depend on c, and $|e^\lambda - 1| \ll |\lambda|$ for λ bounded; note also that $\nu' > \alpha$. Since $(\alpha - 1)/\nu' = \delta/\nu$, we obtain (7) as required, *in the special case where* $E = \mathbb{C}$.

Now let E be a general Banach space. A standard Closed Graph Theorem argument shows that

$$\left(\int_{c+i\mathbb{R}} \frac{|\varphi(F(z))|^\nu}{|z|^{1-\delta}} dy\right)^{1/\nu} \leqslant K\|\varphi\|_{E^*}$$

for all $\varphi \in E^*$, with some constant $K < \infty$. For each $\varphi \in E^*$ we consider $\varphi(F(z))$ and apply the scalar–valued case, to obtain a continuous $g_\varphi : \mathbb{R} \to \mathbb{C}$ such that

$$\varphi(F(z)) = z\mathcal{L}g_\varphi(z), \qquad g_\varphi(t) = \frac{1}{2\pi i}\int_{c+i\mathbb{R}} \frac{\varphi(F(z))}{z} e^{zt}\, dz.$$

Examining the above proof carefully, we find that the constant M in (6) is bounded by an absolute constant multiple of

$$\int_{c+i\mathbb{R}} \frac{|\varphi(F(z))|}{|z|}\,|dz| + \sup_{z\in\Omega} |\varphi(F(z))| \ll \|\varphi\|_{E^*}.$$

Thus $|g_\varphi(t)| \leqslant M'\|\varphi\|_{E^*}(1+t)$ with some $M' < \infty$ for $t > 0$, and similarly for $t < 0$, so we can define $g : \mathbb{R} \to E^{**}$ by $g(t)(\varphi) = g_\varphi(t)$. As usual, regard $E \subseteq E^{**}$ via the canonical embedding. We also have a similar estimate to (7) for

$$g_\varphi(t+s) - g_\varphi(s) = [g(t+s) - g(s)](\varphi),$$

which gives (7) with $\|g(t+s) - g(s)\|_{E^{**}}$ instead of $\|\cdot\|_E$. Crucially, this also shows that $g : \mathbb{R} \to E^{**}$ is *continuous*.

But now $\varphi(F(z)) = z(\mathcal{L}g_\varphi)(z) = [z\mathcal{L}g(z)](\varphi)$, so that $F(z) = z\mathcal{L}g(z)$, considered as an E^{**}-valued function; note that $\mathcal{L}g$ converges because we have an estimate for $\|g(t)\|_{E^{**}}$. Thus all is finished, except that $g(t) \in E^{**}$ instead of E. Put

$$H : \mathbb{R} \to E, \qquad H(t) = \frac{1}{2\pi i}\int_{c+i\mathbb{R}} \frac{F(z)}{z^2} e^{zt}\, dz,$$

which is well–defined and continuous because $\int_{c+i\mathbb{R}} \frac{\|F(z)\|_E}{|z|^2}|dz| < \infty$. Now $(\varphi \circ H)'(t) = (\varphi \circ g)(t)$ for each $\varphi \in E^*$ and $t \in \mathbb{R}$. Because g, $\varphi \circ g$ are continuous, we have

$$\varphi(H(t)) - \varphi(H(0)) = \int_0^t \varphi(g(\tau))\, d\tau.$$

Hence $H(t) = H(0) + \int_0^t g(\tau)\, d\tau$ as an E^{**}-valued integral, so $H'(t) = g(t)$ for all $t \in \mathbb{R}$, again by continuity of $g : \mathbb{R} \to E^{**}$. Thus finally $g(t) \in E$ as required, because H is E-valued.

6 Proof of Theorem 3.2

Now $F : \mathbb{C}_+ \to E$ is *harmonic*; so there exist *analytic* $F_j \in \mathrm{Hol}(\mathbb{C}_+, E)$, with $j = 1, 2$, such that $F(z) = F_1(z) + F_2(\bar{z})$. The functions F_1, F_2 are unique up to additive constants. We will show that F_1, F_2 can be chosen to satisfy (5) in Theorem 3.1, and that F_1, F_2 are almost bounded (*with only logarithmic unboundedness*); the result will then follow by a similar proof to Theorem 3.1.

F is bounded, so we can represent F on $\{\mathrm{Re}(z) > c\}$ by its Poisson integral:

$$\forall\, u > 0, \quad F(c + u + iv) = \frac{1}{\pi} \int_{-\infty}^{\infty} F(c + iy) \frac{u}{u^2 + (v - y)^2}\, dy.$$

Now we define

$$G_1(\lambda) = \frac{1}{2\pi i} \int_{c+i\mathbb{R}} \frac{F(z)}{\lambda - z}\, dz, \qquad G_2(\lambda) = \frac{1}{2\pi i} \int_{c+i\mathbb{R}} \frac{F(z)}{\lambda - \bar{z}}\, dz$$

for all $\mathrm{Re}(\lambda) > c$, so that

$$G_j \in \mathrm{Hol}(\{\mathrm{Re}(\lambda) > c\}, E), \qquad F(\lambda) = G_1(\lambda) + G_2\left(\bar{\lambda}\right).$$

Because $(G_1 - F_1)(\lambda) = -(G_2 - F_2)(\bar{\lambda})$ on $\mathrm{Re}(\lambda) > c$, the functions $G_1 - F_1 \equiv F_2 - G_2$ are constant; so we have analytic continuations $G_j \in \mathrm{Hol}(\mathbb{C}_+, E)$ for $j = 1, 2$.

We use the standard theory of the Weighted Hilbert Transform, found in [22], [16] and many other sources. The famous *Muckenhoupt weight condition* $w \in A_\nu(\mathbb{R})$ for $w : \mathbb{R} \to [0, +\infty]$, $1 < \nu < \infty$ is

$$\sup_{\text{bounded intervals } I \subset \mathbb{R}} \left(\frac{1}{|I|} \int_I w(t)\, dt \right) \left(\frac{1}{|I|} \int_I w(s)^{-1/(\nu-1)}\, ds \right)^{\nu - 1} < \infty.$$

Now $w \in A_\nu(\mathbb{R})$ is *equivalent* to the Hilbert transform being bounded on $L^\nu(w)$:

$$\mathcal{H}f(t) = \lim_{\varepsilon \to 0^+} \frac{1}{\pi} \int_{y \in \mathbb{R},\ |y - t| > \varepsilon} \frac{f(y)}{t - y}\, dy \quad \text{exists for a.e. } t \in \mathbb{R},$$

whenever $f \in L^\nu(w)$, i.e. $\int_{\mathbb{R}} |f|^\nu w\, dt < \infty$, and furthermore $\|\mathcal{H}f\|_{L^\nu(w)} \leqslant C_w \|f\|_{L^\nu(w)}$ for some constant $C_w < \infty$ depending only on w.

For our problem, we easily check that $w(y) = |y|^{-\varsigma}$ satisfies $w \in A_\nu(\mathbb{R})$ for any $0 < \varsigma < 1$. Assume for the moment that $E = \mathbb{C}$. Define

$$H_\varepsilon(\alpha) = \int_{|y - \alpha| > \varepsilon} \frac{F(c + iy)}{\alpha - y}\, dy,$$

so that by above $H_\varepsilon(\alpha) \to H(\alpha)$ as $\varepsilon \to 0$, for almost every $\alpha \in \mathbb{R}$ and some $H \in L^\nu(|\alpha|^{-(1-\delta)})$. Fix $\alpha \in \mathbb{R}$ such that $H_\varepsilon(\alpha) \to H(\alpha)$ does hold. For R large, the condition (5) gives $\int_{|y| > R} \frac{|F(c+iy)|}{|y|}\, dy \ll R^{-\eta}$, and so

$$H_\varepsilon(\alpha) = \int_{\varepsilon < |y - \alpha| < R} \frac{F(c + iy)}{\alpha - y}\, dy + O(R^{-\eta})$$

as $R \to \infty$, for some unimportant $\eta > 0$. But F is harmonic and thus smooth on $\mathbb{C}_+$, so $\int_{|y-\alpha|<1} \left| \frac{F(c+iy)-F(c+i\alpha)}{\alpha-y} \right| dy < \infty$. Also $\int_{\varepsilon<|y-\alpha|<R} \frac{dy}{\alpha-y} = 0$, so we can write

$$\begin{aligned} H_\varepsilon(\alpha) &= \int_{\varepsilon<|y-\alpha|<R} \frac{F(c+iy)-F(c+i\alpha)}{\alpha-y}\, dy + O(R^{-\eta}) \\ &= \int_{|y-\alpha|<R} \frac{F(c+iy)-F(c+i\alpha)}{\alpha-y}\, dy + o_R + o_\varepsilon \end{aligned}$$

where $o_\varepsilon \to 0$ as $\varepsilon \to 0^+$, uniformly in $R > 1$, and similarly $o_R \to 0$ as $R \to \infty$, uniformly in $0 < \varepsilon < 1$. Now, for all $0 < \xi < 1$,

$$\begin{aligned} G_1(c+i\alpha+\xi) &= \frac{1}{2\pi} \int_{|y-\alpha|<R} \frac{F(c+iy)}{\xi+i(\alpha-y)}\, dy + O(R^{-\eta}) \\ &= \frac{1}{2\pi} \int_{|y-\alpha|<R} \frac{F(c+iy)-F(c+i\alpha)}{\xi+i(\alpha-y)}\, dy + o_R \\ &\quad + F(c+i\alpha) I(R,\xi), \end{aligned}$$

where

$$I(R,\xi) = \frac{1}{2\pi} \int_{|y-\alpha|<R} \frac{dy}{\xi+i(\alpha-y)} = \frac{\tan^{-1}(R/\xi)}{\pi}.$$

Now fix R and let $\xi \to 0^+$. Then $I(R,\xi) \to \frac{1}{2}$ and $G_1(c+\xi+i\alpha) \to G_1(c+i\alpha)$, simply because $G_1 \in \mathrm{Hol}(\mathbb{C}_+)$, so that

$$G_1(c+i\alpha) = \frac{1}{2} F(c+i\alpha) + \frac{1}{2\pi i} H_\varepsilon(\alpha) + o_R + o_\varepsilon$$

by Dominated Convergence, because $\int_{|y-\alpha|<R} \left| \frac{F(c+iy)-F(c+i\alpha)}{\alpha-y} \right| dy < \infty$. Finally let $\varepsilon \to 0$ and $R \to \infty$, to give $G_1(c+i\alpha) = \frac{1}{2} F(c+i\alpha) + \frac{1}{2\pi i} H(\alpha)$. This is true for almost every α, and $F(c+i\alpha)$, $H(\alpha)$ are both in $L^\nu(|\alpha|^{-(1-\delta)})$, and thus so is $G_1(c+i\alpha)$.

Now we have $\int_{c+i\mathbb{R}} \frac{|G_1|^\nu}{|z|^{1-\delta}} dy < \infty$, in the special case $E = \mathbb{C}$. In general, we get the same for $\varphi \circ G_1$, for each $\varphi \in E^*$. This is the estimate (5) we need in Theorem 3.1, for G_1 instead of F.

Theorem 3.1 does not apply to G_1 because G_1 may be unbounded. However, the unboundedness is at most *logarithmic*, by two simple calculations:

LEMMA 6.1 *Let $F : \Omega \to E$ be harmonic, for some domain Ω. Then, for every $z \in \Omega$ and $r > 0$ such that $\{\lambda : |\lambda - z| \leqslant r\} \subset \Omega$, we have*

$$\frac{\partial F}{\partial z} = \frac{1}{2\pi i} \oint_{|\lambda-z|=r} \frac{F(\lambda)}{(\lambda-z)^2} d\lambda, \qquad \left\| \frac{\partial F}{\partial z} \right\| \leqslant \frac{\max_{|\lambda-z|=r} \|F(\lambda)\|}{r}.$$

The proof is immediate, from power series representations.

LEMMA 6.2 *Let $F : \mathbb{C}_+ \to E$ be harmonic and bounded, with $F(z) = G_1(z) + G_2(\bar{z})$ for $G_1, G_2 \in \mathrm{Hol}(\mathbb{C}_+, E)$. Then there exist constants $M_j < \infty$, $j = 1, 2$, such that*

$$\|G_j(x+iy)\|_E \leqslant M_j\big(1 + |\log x| + \log(1+|y|)\big). \tag{12}$$

PROOF: Given $u + iv \in \mathbb{C}_+$, we have

$$G_j(u+iv) - G_j(1) = \left(\int_{\substack{x\in[1,S],\\ y=0}} + \int_{\substack{x=S,\\ y\in[0,v]}} + \int_{\substack{x\in[S,u],\\ y=v}}\right) G_j'(z)\,dz,$$

for any $S > 1$. But $G_1' = \partial F/\partial z$, so with $r = x/2$ in Lemma 6.1 we obtain $\|G_1'(x+iy)\| \leqslant 2\left(\sup_{\mathbb{C}_+}\|F\|\right)/x$. Thus

$$\|G_1(u+iv)\| \leqslant \|G_1(1)\| + 2\sup_{\mathbb{C}_+}\|F\|\left(\log S + \frac{|v|}{S} + |\log S - \log u|\right).$$

Now letting $S = |v| + 1$ gives the result for G_1, and the proof for G_2 is similar. □

The logarithmic terms are unavoidable; e.g. $2\theta = -i(\log z - \log\bar{z})$ is harmonic and bounded on $\mathbb{C}_+ = \{re^{i\theta} : r > 0, |\theta| < \pi/2\}$.

Finally, to complete the proof of Theorem 3.2: G_1 satisfies (12), and also the vertical estimate (5) on $c + i\mathbb{R}$. Similarly, or by considering $F(\bar{z})$ instead, G_2 also satisfies the same estimates. The local Hölder estimate (7) follows from the proof of Theorem 3.1 without change, since only (5) is needed.

To estimate $\|g_j(t)\|$ for large $t > 0$, we use the same method as Theorem 3.1 (which in fact is the method used in [3]), but with additional logarithmic estimates. As usual, consider $\varphi \circ F$ for each $\varphi \in E^*$. In the contour integral formula

$$\varphi \circ g_j(t) = \frac{1}{2\pi i}\int_{c+i\mathbb{R}} \frac{\varphi \circ G_j(z)}{z} e^{zt}\,dz,$$

use Cauchy's Theorem to replace $c + i\mathbb{R}$ by the contours $\{c + iy : |y| \geqslant \kappa\}$, $\{x \pm i\kappa : t^{-1} < x < c\}$ and $\{t^{-1} + iy : |y| \leqslant \kappa\}$, for t large. Estimating $\left|\frac{\varphi\circ G_j(z)}{z}e^{zt}\right|$ on each of these contours finally gives that $|\varphi \circ g_j(t)|/\|\varphi\|_{E^*}$ is

$$\ll e^{ct}\kappa^{-\epsilon} + (1 + \log t + \log(1+\kappa))\big[e^{ct}\kappa^{-1} + \exp(t^{-1}\cdot t)\log(\kappa t)\big]$$

for t large and some $0 < \epsilon < 1$, which is $\ll t^2$ upon taking $\kappa = \exp(ct/\epsilon)$.

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Local Classes and Pairwise Mutually Permutable Products of Finite Groups

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Abstract. The main aim of the paper is to present some results about products of pairwise mutually permutable subgroups and local classes.

Keywords and Phrases: mutually permutable, local classes, p-soluble groups, p-supersolubility, finite groups

1 Introduction

If A and B are subgroups of a group G, the product AB of A and B is defined to be the subset of all elements of G with the form ab, where $a \in A, b \in B$. It is well known that AB is a subgroup of G if and only if $AB = BA$, that is, if the subgroups A and B permute. Should it happen that AB coincides with the group G, with the result that $G = AB = BA$, then G is said to be factorized by its subgroups A and B. More generally, a group G is said to be the product of its pairwise permutable subgroups $G_1, G_2, \ldots, G_n$ if $G = G_1G_2 \ldots G_n$ and $G_iG_j = G_jG_i$ for all integers i and j with $i, j \in \{1, 2, \ldots, n\}$. This implies that for every choice of indices $1 \leq i_1 \leq i_2 \leq \ldots \leq i_k \leq n$, the product $G_{i_1}G_{i_2} \ldots G_{i_k}$ is a subgroup of G. Groups which are product of two of its subgroups have played a significant part in the theory of groups over the past sixty years. Among the central problems considered the following ones are of interest to us:

Let the group $G = G_1G_2 \ldots G_n$ be the product of its pairwise permutable subgroups $G_1, G_2, \ldots, G_n$ and suppose that the factors G_i, $1 \leq i \leq n$, belong to a class of groups $\mathcal{X}$. When does the group G belong to $\mathcal{X}$?. How does the *structure of the factors G_i, $1 \leq i \leq n$ affect the structure of the group G?.*

Obviously, if G_i, $1 \leq i \leq n$, are finite, then the group G is finite. However not many properties carry over from the factors of a factorized group to the group itself. Indeed if one thinks about properties such as solubility, supersolubility, or nilpotency, one soon realizes the difficulty of using factorization to obtain information about the structure of the whole group. Two well known examples support the above claim: there exist non abelian groups which are products of two abelian subgroups and every finite soluble group is the product of pairwise permutable nilpotent subgroups. However a prominent result by Itô shows that every product of two abelian groups is metabelian, and an important result of Kegel and Wielandt shows the solubility of every finite group $G = G_1 G_2 \dots G_n$ which is the product of pairwise permutable nilpotent subgroups G_i, $1 \leq i \leq n$. In the much more special case when G_i, $1 \leq i \leq n$, are normal nilpotent subgroups of G, the product $G_1 G_2 \dots G_n$ is nilpotent. This is a well known result of Fitting. However, if $G_1, G_2, \dots, G_n$ are normal supersoluble subgroups of G, the product $G_1 G_2 \dots G_n$ is not supersoluble in general even in the finite case (see [1]). Consequently it seems reasonable to look into these problems under additional assumptions. In this context, assumptions on permutability connections between the factors turn out to be very useful. One of the most important ones is the mutual permutability introduced by Asaad and Shaalan in [1]. We say that two subgroups A and B of a group G are mutually permutable if A permutes with every subgroup of B and B permutes with every subgroup of A. If $G = AB$ and A and B are mutually permutable, then G is called a mutually permutable product of A and B. More generally, a group $G = G_1 G_2 \dots G_n$ is said to be the product of the pairwise mutually permutable subgroups $G_1, G_2, \dots, G_n$ if G_i and G_j are mutually permutable subgroups of G for all $i, j \in \{1, 2, \dots, n\}$. Asaad and Shaalan ([1]) proved that if G is a mutually permutable product of the subgroups A and B and A and B are finite and supersoluble, then G is supersoluble provided that either G', the derived subgroup of G, is nilpotent or A or B is nilpotent. This result was the beginning of an intensive study of such factorized groups (see, for instance, [2, 4, 6, 9] and the papers cited therein).

The extension of the above results on mutually permutable products of two subgroups to general pairwise mutually permutable products turns out to be difficult in many cases. Carocca proved (see [10]) that if the derived subgroup of a pairwise mutually permutable product of supersoluble subgroups is nilpotent, then the group G is supersoluble. However a pairwise mutually permutable product of supersoluble groups in which one of them is nilpotent is not supersoluble in general (see [4, Example]). Nevertheless in [4] we obtained that if G is the pairwise mutually permutable product of supersoluble subgroups with all factors but one nilpotent, then the group is supersoluble.

Some interesting results on pairwise mutually permutable products arise when the factors belong to some classes of finite groups which are defined in terms of permutability. They are the class of PST-groups, or finite groups G in which every subnormal subgroup of G permutes with every Sylow subgroup of G, the class of PT-groups, or finite groups in which every subnormal subgroup is a permutable subgroup of the group, the class of T-groups, or groups in which every subnormal subgroup is normal, and the class of $\mathcal{Y}$-groups, or finite groups G for which for every subgroup H and for all primes q dividing the index $|G : H|$ there exists a subgroup K of G such that H is contained in K and $|K : H| = q$, and their corresponding local versions (see [2, 3]).

The main purpose of this article is to take this program of research a step further by analyzing the structure of the pairwise mutually permutable products whose factors belong to some local classes of finite groups closely related to the classes of all T-groups and $\mathcal{Y}$-groups.

Therefore in the sequel all groups considered are finite.

2 The class $\bar{\mathcal{C}_p}$ and pairwise mutually permutable products

Throughout this section, p will be a prime.
Recall that a group G satisfies property $\mathcal{C}_p$, or G is a $\mathcal{C}_p$-group, if each subgroup of a Sylow p-subgroup P of G is normal in the normalizer $N_G(P)$. This class of groups was introduced by Robinson in his seminal paper [14] as a local version of the class of all soluble T-groups. In fact, he proved there that a group G is a soluble T-group if and only if G is a $\mathcal{C}_p$-group for all primes p.
In [7] the second and third authors introduce and analyze an interesting class of groups closely related to the class of all T-groups. A group G is a T_1-group if $G/Z_\infty(G)$ is a T-group. Here $Z_\infty(G)$ denotes the hypercenter of G, that is, the largest normal subgroup of G having a G-invariant series with central G-chief factors. The local version of the class T_1 in the soluble universe is the class $\bar{\mathcal{C}_p}$ introduced and studied in [8]:

Definition 1. *Let G be a group and let $Z_p(G)$ be the Sylow p-subgroup of $Z_\infty(G)$. A group satisfies $\bar{\mathcal{C}_p}$ if and only if $G/Z_p(G)$ is a $\mathcal{C}_p$-group.*

Theorem A ([8]) *A group G is a soluble T_1-group if and only if G is a $\bar{\mathcal{C}_p}$-group for all primes p.*

The objective of this section is to analyze the behaviour of pairwise mutually permutable products with respect to the class $\bar{\mathcal{C}_p}$.

We begin with some results concerning the classes $\mathcal{C}_p$ and $\bar{\mathcal{C}_p}$.

Lemma 1. *[8, Lemma 2] Let p be a prime. Then:*

(i) $\mathcal{C}_p$ is a subgroup-closed class.

(ii) Let M be a normal p'-subgroup of a group G. If G/M is a $\mathcal{C}_p$-group, then so is G.

(iii) If G is a $\mathcal{C}_p$-group and N is a normal subgroup of G, then G/N is a $\mathcal{C}_p$-group.

Lemma 2. *Let G be a $\bar{\mathcal{C}}_p$-group and let N be a normal subgroup of G. Then G/N is a $\bar{\mathcal{C}}_p$-group.*

Proof Let $Z_p(G)$ be the Sylow p-subgroup of $Z_\infty(G)$. Since $G/Z_p(G)$ is a $\mathcal{C}_p$-group, it follows that $G/Z_p(G)N$ is a $\mathcal{C}_p$-group by Lemma 1. Let H/N denote the Sylow p-subgroup of $Z_\infty(G/N)$. Since $Z_p(G)N/N$ is contained in H/N, we have that $(G/N)/(H/N)$ is isomorphic to a quotient of $G/Z_p(G)N$. By Lemma 1, $(G/N)/(H/N)$ is a $\mathcal{C}_p$-group. Therefore G/N is a $\bar{\mathcal{C}}_p$-group.

Recall that a group G is said to be p-supersoluble if it is p-soluble and every p-chief factor of G is cyclic. It is rather clear that the derived subgroup of a p-supersoluble group is p-nilpotent and, if $p = 2$, the group itself is 2-nilpotent.

Lemma 3. *[8, Lemma 3] Let G be a p-soluble group. If G is a $\bar{\mathcal{C}}_p$-group, then G is p-supersoluble.*

The main aim of this section is to show that pairwise mutually permutable products of p-soluble $\bar{\mathcal{C}}_p$-groups are p-supersoluble.

Theorem 1. *Let $G = G_1G_2 \ldots G_k$ be the pairwise mutually permutable product of the subgroups $G_1, G_2, \ldots, G_k$. If G_i is a p-soluble $\bar{\mathcal{C}}_p$-group for every $i \in \{1, 2, \ldots, k\}$, then G is p-supersoluble.*

Proof Assume that the theorem is false, and let G be a counterexample with minimal order. By [4, Theorem 1], G is p-soluble. If $p = 2$, then G_i is 2-nilpotent for all $i = 1, 2, \ldots, k$ and so G is 2-supersoluble by [4, Theorem 3]. This contradiction implies that p is odd. Note, that the hypotheses of the theorem are inherited by all proper quotients of G. Therefore the minimal choice of G yields G/N p-supersoluble for every minimal normal subgroup N of G. Since the class of p-supersoluble groups is a saturated formation, it follows that G has a unique minimal normal subgroup, say N, G/N is p-supersoluble, the Frattini subgroup of G is trivial and then $N = C_G(N) = F(G) = O_p(G)$. Moreover, N is an elementary abelian p-group of rank greater than 1.
By Lemma 3, G_i is p-supersoluble, for all $i = 1, 2, \ldots, k$. Consequently $(G_i)'$ is p-nilpotent. Furthermore, by [4, Lemma 1(iii)], we have that $(G_i)'$ is a subnormal subgroup of G for all i. Since $O_{p'}(G) = 1$, it follows that $(G_i)'$ is a p-group and then G_i is supersoluble for all i. Then G_i is a Sylow tower group with respect to the reverse natural ordering of the prime numbers for all i. Applying [4, Corollary 1], G is a Sylow tower group with respect to the reverse natural ordering of the prime numbers. Therefore p is the largest prime dividing the order of G and $F(G) = N$ is the Sylow p-subgroup of G.
Now we observe the following facts:

(i) For each $i \in \{1, 2, \ldots, k\}$, either $N \leq G_i$ or $N \cap G_i = 1$.
Put $R := N \cap G_i$, and assume that $R \neq 1$. Let H_j be a Hall p'-subgroup of

G_j (such Hall subgroups exist since G_j is soluble). Then $R = G_iH_j \cap N$, so $G_j \leq NH_j \leq N_G(R)$ for every j. Hence R is a normal subgroup of G and $R = N$.

(ii) Let $N \leq G_i$, with $i \in \{1, 2, \ldots, k\}$. Then $Z_\infty(G_i) = Z(G_i)$, $N = Z(G_i) \times [N, G_i]$, and every subgroup of $[N, G_i]$ is G_i-invariant.
Clearly $N \leq F(G_i)$ and $O_{p'}(F(G_i)) \leq C_G(N) = N$. Thus $F(G_i) = N$. Therefore $Z_\infty(G_i) \leq N$, and $Z_\infty(G_i) = Z(G_i)$, since $G_i/C_{G_i}(Z_\infty(G_i))$ is a p-group (G_i stabilizes a series of subgroups of $Z_\infty(G_i)$, see [11, A, 12.4]) and N is a Sylow p-subgroup of G_i. Moreover, $N = Z(G_i) \times [N, G_i]$ since G_i/N is a p'-group. As $G_i \in \bar{\mathcal{C}}_p$ and $Z(G_i) = Z_\infty(G_i)$, G_i normalizes every subgroup of $[N, G_i]$.

(iii) Let $N \leq G_i$ with $i \in \{1, 2, \ldots, k\}$, then every $y \in G_i \setminus N$ induces a non-trivial $GF(p)$-scalar multiplication on $[N, G_i]$; in particular $C_N(y) = Z(G_i)$ and G_i/N is cyclic.
Note that G/N acts faithfully on N. So y induces a non-trivial linear mapping on the $GF(p)$-space $[N, G_i]$ that leaves invariant every subspace. It is well-known that these mappings come from multiplication with an element of $GF(p)$.

(iv) Let $N \leq G_i$ and $N \leq G_j$ with $i \in \{1, 2, \ldots, k\}$. Suppose that $N_{G_i}(Z(G_j)) \not\leq N$. Then $G_i \leq N_G(Z(G_j))$.
Put $R := N_{G_i}(Z(G_j))$. By (iii), $Z(G_j) = (Z(G_j) \cap Z(G_i)) \times [Z(G_j), R]$, and $[Z(G_j), R] \leq [N, G_i]$. Thus by (ii), $Z(G_j)$ is G_i-invariant.

(v) Suppose that $N \leq G_i$ and $G_j \leq N_G(Z(G_i))$. Then $[G_i, G_j] \leq N$; in particular, if $N \leq G_j$, $G_i \leq N_G(Z(G_j))$.
Put $H := G_iG_j$. Then H/N is a p'-group. By Maschke's Theorem there exists an H-invariant complement N_0 for $Z(G_i)$ in N. By (iii) $N_0 = [N, G_i]$ and $[G_i, G_j] \leq C_H(N_0)$. Since also $[G_i, G_j] \leq C_H(Z(G_i))$, it follows that $[G_i, G_j] \leq C_H(N) \leq N$. Moreover if $N \leq G_j$ we have that $G_j^H = G_j^{G_i} = G_j[G_i, G_j] = G_j$, that is, G_j is a normal subgroup of H and then G_i normalizes $Z(G_j)$.

(vi) Let $R \leq N \cap G_i$ and $G_j \cap N = 1$. Then G_j normalizes R.
Since RG_j is a subgroup of G, $RG_j \cap N = R$ is a normal subgroup of RG_j.

(vii) Suppose that $N \leq G_j$. Then $Z(G_j)$ is a normal subgroup of G.
We may assume that there exists $i \in \{1, 2, \ldots, k\}$ such that $G_i \not\leq N_G(Z(G_j))$. In particular $Z(G_j) \neq 1$, and $Z(G_j) \leq N$ by (ii). Now the application of (vi) yields $G_i \cap N \neq 1$ and so by (i) also $N \leq G_i$. Moreover, $G_i \notin \mathcal{C}_p$ and so $Z_\infty(G_i) \neq 1$. Applying (ii) $Z_\infty(G_i) = Z(G_i) \neq 1$, and by (v) $G_j \not\leq N_G(Z(G_i))$. Hence the situation is completely symmetric in i and j.
Put $H := G_iG_j$. We first show:

(*) $G_i \cap G_j = N$, and $N_H(RN) = G_k$ for every $k \in \{i, j\}$ and $R \leq G_k$ with $R \nleq N$.
Since G_k/N is cyclic by (iii), RN is a normal subgroup of G_k and so $N_H(RN) = N_{G_t}(RN)G_k$, where $\{t, k\} = \{i, j\}$. Now (iv) yields $N_{G_t}(RN) \leq N$. This shows that $G_i \cap G_j = N$ and $N_H(RN) = G_k$.
As a consequence of (*), G_i/N and G_j/N have trivial intersection, therefore $H/N = (G_i/N)(G_j/N)$ is the totally permutable product of G_i/N and G_j/N (see [6, Lemma 1]), that is, every subgroup of G_i/N permutes with every subgroup of G_j/N. Thus there exists RN/N a minimal normal subgroup of H/N contained in G_i/N or in G_j/N (see [10]), suppose $RN/N \leq G_i/N$ without loss of generality. Then $N_H(RN) = H$. On the other hand, by (*) $N_H(RN) = G_i$. But then $G_j \leq G_i$, a contradiction since $G_j \nleq N_G(Z(G_i))$.

Since not all the factors G_i are p'-groups, there exists G_i with $N \leq G_i$. It suffices to show that every subgroup R of N is normal in G. By (i) and (vi) every G_j with $N \nleq G_j$ normalizes R. On the other hand, by (vii) for every G_j with $N \leq G_j$ either $N = Z(G_j) = G_j$ or $Z(G_j) = 1$. In the first case obviously $G_j \leq N_G(R)$. In the second case $G_j \in \mathcal{C}_p$ and again $G_j \leq N_G(R)$. Consequently $\mid N \mid = p$, the final contradiction.

Combining Theorems A and 1 we have:

Corollary 1. *Let $G = G_1G_2 \dots G_k$ be a product of the pairwise mutually permutable soluble T_1-groups $G_1, G_2, \dots, G_k$. Then G is supersoluble.*

3 The class $\hat{\mathcal{Z}}_p$ and pairwise mutually permutable products

Another interesting class of groups closely related to T-groups is the class T_0 of all groups G whose Frattini quotient $G/\Phi(G)$ is a T-group. This class was introduced in [15] and studied in [12, 13, 15].
The procedure of defining local versions in order to simplify the study of global properties has also been successfully applied to the study of the classes T_0 ([12]) and $\mathcal{Y}$ ([3]).

Definition 2. *Let p be a prime and let G be a group.*

(i) ([12]) Let $\Phi(G)_p$ be the Sylow p-subgroup of the Frattini subgroup of G. G is said to be a $\hat{\mathcal{C}}_p$-group if $G/\Phi(G)_p$ is a $\mathcal{C}_p$-group.

(ii) ([3, Definition 11]) We say that G satisfies $\mathcal{Z}_p$ or G is a $\mathcal{Z}_p$-group when for every p-subgroup X of G and for every power of a prime q, q^m, dividing $\mid G : XO_{p'}(G) \mid$, there exists a subgroup K of G containing $XO_{p'}(G)$ such that $\mid K : XO_{p'}(G) \mid= q^m$.

It is rather clear that the class of all $\hat{\mathcal{C}}_p$-groups is closed under taking epimorphic images and all p-soluble groups belonging to $\hat{\mathcal{C}}_p$ are p-supersoluble. Moreover:

THEOREM B ([12]) *A group G is a soluble T_0-group if and only if G is a $\hat{\mathcal{C}}_p$-group for all primes p.*

In the following two results we gather some useful properties of the $\mathcal{Z}_p$-groups.

LEMMA 4. *Let G be a group.*

(i) If G is a p-soluble $\mathcal{Z}_p$-group, then G is p-supersoluble. [3, Lemma 20]

(ii) If G is a p-soluble $\mathcal{Z}_p$-group and N is a normal subgroup of G, then G/N is a $\mathcal{Z}_p$-group. [3, Lemma 18]

(iiii) Let G be a soluble group. G is a $\mathcal{Y}$-group if and only if G is a $\mathcal{Z}_p$-group for every prime p. [3, Theorem 15]

THEOREM C [3, Theorem 13] *Let p be a prime and G a p-soluble group. Then G satisfies $\mathcal{Z}_p$ if and only if G satisfies one of the following conditions:*

(1) G is p-nilpotent.

(2) $G(p)/O_{p'}(G(p))$ is a Sylow p-subgroup of $G/O_{p'}(G(p))$ and for every p-subgroup H of $G(p)$, we have that $G = N_G(H)G(p)$.

Here $G(p)$ denotes the p-nilpotent residual of G, that is, the smallest normal subgroup of G with p-nilpotent quotient.

The results of [5] show that the class $\mathcal{C}_p$ is a proper subclass of the class $\mathcal{Z}_p$.

In [2, Theorem 16] it is proved that a pairwise mutually permutable product of $\mathcal{Y}$-groups is supersoluble. There it is asked whether a pairwise mutually permutable product of $\mathcal{Z}_p$-groups is p-supersoluble. In this section, we answer to this question affirmatively. In fact, the main purpose here is to study pairwise mutually permutable products whose factors belong to some class of groups closely related to $\mathcal{Z}_p$-groups.

DEFINITION 3. *Let p be a prime, let G be a group and let $\Phi(G)_p$ be the Sylow p-subgroup of the Frattini subgroup of G. G is said to be a $\hat{\mathcal{Z}}_p$-group if $G/\Phi(G)_p$ is a $\mathcal{Z}_p$-group.*

LEMMA 5. *Let p be a prime and M a normal subgroup of G. If G is a $\hat{\mathcal{Z}}_p$-group, then G/M is a $\hat{\mathcal{Z}}_p$-group.*

PROOF Assume that G is a $\hat{\mathcal{Z}}_p$-group. Then $G/\Phi(G)_p$ is a $\mathcal{Z}_p$-group. Since $\Phi(G)_pM/M$ is contained in $\Phi(G/M)_p = L/M$ and the class of all $\mathcal{Z}_p$-groups is closed under taking epimorphic images, we have that G/L belongs to $\mathcal{Z}_p$. This is to say that G/M is a $\hat{\mathcal{Z}}_p$-group.

Since the class of all p-supersoluble groups is a saturated formation and, by Lemma 4(i), every p-soluble $\mathcal{Z}_p$-group is p-supersoluble, we have:

Lemma 6. *Let p be a prime and let G be a p-soluble group. If G is a $\hat{\mathcal{Z}}_p$-group, then G is p-supersoluble.*

The main result of this section shows that pairwise mutually permutable products of $\hat{\mathcal{Z}}_p$-groups are p-supersoluble.

Theorem 2. *Let $G = AB$ be the mutually permutable product of the p-supersoluble group A and the p-soluble $\hat{\mathcal{Z}}_p$-group B. Then G is p-supersoluble.*

Proof Assume that the result is false, and let G be a counterexample of minimal order. Applying [4, Theorem 1], G is p-soluble. Let N be a minimal normal subgroup of G. Then G/N is the mutually permutable product of the subgroups AN/N and BN/N. Moreover, AN/N is p-supersoluble and BN/N is a p-soluble $\hat{\mathcal{Z}}_p$-group by Lemma 5. The minimality of G implies that G/N is p-supersoluble. Since p-supersoluble groups is a saturated formation, it follows that G has a unique minimal normal subgroup, N say. Moreover N is an elementary abelian p-group of rank greater than 1 and $N = C_G(N) = F(G) = O_p(G)$. Note further that, by Lemma 6, A and B are p-supersoluble.
Applying [6, Lemma 1(vii)], we have that A and B either cover or avoid N. If A and B both avoid N, then $|N| = p$ by [6, Lemma 2] and G is p-supersoluble. This contradiction allows us to assume that $N \leq A$. Suppose that $B \cap N = 1$ and let X be a minimal normal subgroup of A such that $X \leq N$. Then $|X| = p$ and $XB \cap N = X$ is a normal subgroup of XB. It means that B normalizes X and so X is a normal subgroup of G. This would imply that G is p-supersoluble, contrary to our supposition. We obtain also a contradiction if we assume $N \leq B$ and $A \cap N = 1$. Therefore we may suppose that $N \leq A \cap B$. Note that, by [4, Theorem 3], neither A nor B is p-nilpotent.
On the other hand, by [6, Theorem 1], we have that A' and B' are subnormal subgroups of G. Since they are p-nilpotent and $O_{p'p}(G) = N$, it follows that $\langle A', B' \rangle \leq N$. Let $1 \neq B(p)$ be the p-nilpotent residual of B. Then $B(p) \leq B' \leq N$. Now observe that $O_{p'}(B) = 1$ and B is p-closed. Then it is an elementary fact that $\Phi(B) = \Phi(O_p(B)) = \Phi(B)_p$. Since B is not p-nilpotent, Theorem C gives $B(p) \in Syl_p(B)$, so $N = B(p)$ and $\Phi(B) = \Phi(N) = 1$. In particular $B \in \mathcal{Z}_p$ and by Theorem C every subgroup of N is normal in B. Therefore, if X is a minimal normal subgroup of A contained in N, we have that X is a normal subgroup of G of order p. Consequently, G is p-supersoluble, the final contradiction.

Theorem 3. *Let $G = G_1 G_2 \dots G_n$ be the pairwise mutually permutable product of the subgroups $G_1, G_2, \dots, G_n$. If G_i is a p-soluble $\hat{\mathcal{Z}}_p$-group for every i, then G is p-supersoluble.*

Proof Assume that the theorem is false, and among the counterexamples with minimal order choose one $G = G_1G_2 \dots G_n$ such that the sum $|G_1| + |G_2| + \dots + |G_n|$ is minimal. By Theorem 2, we have $n > 2$. Moreover, by [4, Theorem 1], G is p-soluble. It is rather clear that the hypotheses of the theorem are inherited by all proper quotients of G. Hence G contains a unique minimal normal subgroup, N say, N is not cyclic, G/N is p-supersoluble and $N = C_G(N) = O_p(G)$. Hence $O_{p'}(G) = 1$. By Lemma 6, G_i is p-supersoluble and hence G_i' is p-nilpotent for every i. Applying Lemma 1(iii) of [4], we have that G_i' is a subnormal subgroup of G for each $i \in \{1, 2, \dots, n\}$. Hence G_i' is contained in N and so G_i is supersoluble for each $i \in \{1, 2, \dots, n\}$. By [4, Corollary 1], G is a Sylow tower group with respect to the reverse natural ordering of the prime numbers, p is the largest prime divisor of $|G|$ and N is the Sylow p-subgroup of G.
Let $i \in \{1, 2, \dots, n\}$ such that p divides $|G_i|$. Then $N \cap G_i$ is the non-trivial Sylow p-subgroup of G_i. Let $j \in \{1, 2, \dots, n\}$ such that $j \neq i$. Then $G_i(G_j)_{p'}$ is a subgroup of G and $N \cap G_i$ is a Sylow p-subgroup of $G_i(G_j)_{p'}$. Since $G_i(G_j)_{p'}$ is a Sylow tower group with respect to the reverse natural ordering of the prime numbers, it follows that $N \cap G_i$ is normal in $G_i(G_j)_{p'}$. This implies that $N \cap G_i$ is a normal subgroup of G and so $N = N \cap G_i$ is contained in G_i.
Assume that there exists $j \in \{1, 2, \dots, n\}$ such that p does not divide $|G_j|$. We may assume without loss of generality $j = 1$. Then $G_1' = 1$, that is, G_1 is an abelian p'-group, and $T = G_2G_3 \dots G_n$ is p-supersoluble by the choice of G. Let R be a minimal normal subgroup of T contained in N. Then $|R| = p$. Moreover, G_1R is a subgroup of G because N is contained in some of the factors G_l, $l > 1$. Hence $G_1R \cap N = R$ is a normal subgroup of G_1R. Hence R is a normal subgroup of G and so $N = R$. This is a contradiction. Therefore p divides the order of G_i for every $i \in \{1, 2, \dots, n\}$. Consequently, N is contained in G_i for every $i \in \{1, 2, \dots, n\}$.
Consider now $W = G_2G_3 \dots G_n$. Then W is p-supersoluble. Let X be a minimal normal subgroup of W contained in N. Then $|X| = p$. Recall that G_1 is a $\hat{\mathcal{Z}}_p$-group. Assume that $G_1/\Phi(G_1)_p$ is p-nilpotent. Then G_1 is p-nilpotent. Since N is self-centralizing in G, it follows that $G_1 = N$. Suppose that $G_1/\Phi(G_1)_p$ satisfies condition (2) of Theorem C. Then we can argue as in the proof of Theorem 2 to obtain that $N = G_1(p)$, the p-nilpotent residual of G_1, and $\Phi(G_1)_p = 1$. Consequently every subgroup of N is normal in G_1. In both cases, we have that G_1 normalizes X. It means that $N = X$, the final contradiction.

Applying Theorems C and 3 we have:

Corollary 2. *Let $G = G_1G_2 \dots G_n$ be a group such that $G_1, G_2, \dots, G_n$ are pairwise mutually permutable subgroups of G. If all G_i are p-nilpotent, then G is p-supersoluble.*

Since every $\mathcal{Z}_p$-group is a $\hat{\mathcal{Z}}_p$-group, we can apply Lemma 4(iii) and Theorem 3 to obtain the following:

Corollary 3. *[2, Theorem 16] Let $G = G_1G_2 \dots G_n$ be a group such that $G_1, G_2, \dots, G_n$ are pairwise mutually permutable subgroups of G. If all G_i are $\mathcal{Y}$-groups, then G is supersoluble.*

Finally, applying Theorems B and 3, we have:

Corollary 4. *Let $G = G_1G_2 \dots G_n$ be a group such that $G_1, G_2, \dots, G_n$ are pairwise mutually permutable subgroups of G. If all G_i are soluble T_0-groups, then G is supersoluble.*

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Blow-up of Solutions to a Periodic Nonlinear Dispersive Rod Equation

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Abstract. In this paper, firstly we find an optimal constant for a convolution problem on the unit circle via the variational method. Then by using the optimal constant, we give a new and improved sufficient condition on the initial data to guarantee the corresponding strong solution blows up in finite time. We also analyze the corresponding ordinary difference equation associate to the convolution problem and give numerical simulation for the optimal constant.

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1 Introduction

Although a rod is always three-dimensional, if its diameter is much less than the axial length scale, one-dimensional equations can give a good description of the motion of the rod. Recently Dai [16] derived a new (one-dimensional) nonlinear dispersive equation including extra nonlinear terms involving second-order and third-order derivatives for a compressible hyperelastic material. The equation reads

$$v_\tau + \sigma_1 v v_\xi + \sigma_2 v_{\xi\xi\tau} + \sigma_3(2v_\xi v_{\xi\xi} + v v_{\xi\xi\xi}) = 0,$$

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where $v(\xi, \tau)$ represents the radial stretch relative to a pre-stressed state, $\sigma_1 \neq 0$, $\sigma_2 < 0$ and $\sigma_3 \leq 0$ are constants determined by the pre-stress and the material parameters. If one introduces the following transformations

$$\tau = \frac{3\sqrt{-\sigma_2}}{\sigma_1} t, \ \ \xi = \sqrt{-\sigma_2} x,$$

then the above equation turns into

$$u_t - u_{txx} + 3uu_x = \gamma(2u_x u_{xx} + uu_{xxx}), \tag{1.1}$$

where $\gamma = 3\sigma_3/(\sigma_1\sigma_2)$. In [17], the authors derived that value range of γ is from -29.4760 to 3.4174 for some special compressible materials. From the mathematical view point, we regard γ as a real number.

When $\gamma = 1$ in (1.1), we recover the shallow water (Camassa-Holm) equation derived physically by Camassa and Holm in [4] (found earlier by Fuchssteiner and Fokas [18] as a bi-Hamiltonian generalization of the KdV equation) by approximating directly the Hamiltonian for Euler's equations in the shallow water region, where $u(x, t)$ represents the free surface above a flat bottom. Recently, the alternative derivations of the Camassa-Holm equation as a model for water waves, respectively as the equation for geodesic flow on the diffeomorphism group of the circle were presented in [27] and respectively in [9, 29]. For the physical derivation, we refer to works in [10, 26]. Some satisfactory results have been obtained for this shallow water equation. Local well-posedness for the initial datum $u_0(x) \in H^s$ with $s > 3/2$ was proved by several authors, see [30, 32, 35]. For the initial data with lower regularity, we refer to [33] and [2]. While the regularized generalized Camassa–Holm equation was analyzed in [15]. Moreover, wave breaking for a large class of initial data has been established in [5, 7, 8, 30, 38, 39]. However, in [37], global existence of weak solutions is proved but uniqueness is obtained only under an a priori assumption that is known to hold only for initial data $u_0(x) \in H^1$ such that $u_0 - u_{0xx}$ is a sign-definite Radon measure (under this condition, global existence and uniqueness was shown in [12] also). Also it is worth to note that the global conservative solutions and global dissipative solutions (with energy being lost when wave breaking occurs) are constructed in [2, 22, 24] and [3, 25]. Recently, in [21], Himonas, Misiołek, Ponce and the third author showed the infinite propagation speed for the Camassa-Holm equation in the sense that a strong solution of the Cauchy problem with compact initial profile can not be compactly supported at any later time unless it is the zero solution, which is an improvement of previous results in this direction obtained in [6].

If $\gamma = 0$, (1.1) is the BBM equation, a well-known model for surface waves in a canal [1], and its solutions are global.

For general $\gamma \in \mathbb{R}$, the rod equation (1.1) was studied sketchily by the Constantin and Strauss in [13] first. Local well-posedness of strong solutions to (1.1) was established by applying Kato's theory [28] and some sufficient conditions on the initial data were found to guarantee the finite blow-up of the corresponding solutions for spatially nonperiodic case. Weak solutions was constructed in [14, 23]. Later, in [41], the third author proved the well-posedness result in detail, and various refined sufficient conditions on the initial data were found to guarantee the finite blow-up of the corresponding solutions for both spatially periodic and nonperiodic cases. Recently, blow-up criteria for a special class of initial data for the periodic rod equation was presented in [31, 42], where $\mathbb{S} = \mathbb{R}/\mathbb{Z}$ is the unit circle. Furthermore, in [20], Guo and the third author have investigated the persistence properties for this rod equation. It should be mentioned that for $\gamma < 1$, (1.1) admits smooth solitary waves observed by Dai and Huo [17]. Let $u(x,t) = \phi(\xi), \xi = x - ct$ be the solitary wave to (1.1). It was shown that $\phi(\xi)$ satisfies

$$\pm\xi = -\sqrt{-\gamma}\left(\frac{1}{2}\pi + \arcsin\frac{2\gamma\phi - (\gamma+1)c}{(1-\gamma)c}\right) - \ln\frac{(\sqrt{c(c-\phi)} + \sqrt{c(c-\gamma\phi)})^2}{(1-\gamma)c\phi}$$

for $\gamma < 0$ and

$$\pm\xi = \sqrt{\gamma}\ln\frac{(\sqrt{c-\gamma\phi)} - \sqrt{\gamma(c-\phi)})^2}{(1-\gamma)c} - \ln\frac{(\sqrt{c-\gamma\phi} + \sqrt{c-\phi})^2}{(1-\gamma)\phi}$$

for $0 < \gamma < 1$. In [13] (see [40] also), Constantin and Strauss proved the stability of these solitary waves by applying a general theorem established by Grillakis, Shatah and Strauss [19].

We conclude this introduction by outlining the rest of the paper. In section 2, we recall the local well-posedness for (1.1) with initial datum $u_0 \in H^s$, $s > 3/2$, and the lifespan of the corresponding solution is finite if and only if its first-order derivative blows up. In section 3, formulation of the optimal constant for a convolution problem is settled by a variational method described in Struwe's book [36]. Then we solve the nonlinear ordinary differential equation in section 4. In section 5, a new blow-up criterion is established by applying the best constant for the convolution problem. Finally, in section 6, another representation will be showed, and a numerical simulation will be given.

2 Preliminaries

In this section, we concentrate on the periodic case. In [13, 41], it is proved that

Theorem 2.1 [13, 41] *Let the initial datum $u_0(x) \in H^s(\mathbb{S})$, $s > 3/2$. Then there exists $T = T(\|u_0\|_{H^s}) > 0$ and a unique solution u, which depends continuously on the initial datum u_0, to (1.1) such that*

$$u \in C\left([0,T); H^s(\mathbb{S})\right) \cap C^1\left([0,T); H^{s-1}(\mathbb{S})\right).$$

Moreover, the following two quantities E and F are invariants with respect to *time t for (1.1).*

$$\begin{cases} E(u)(t) = \int_{\mathbb{S}} \left(u^2(x,t) + u_x^2(x,t)\right) dx, \\ F(u)(t) = \int_{\mathbb{S}} \left(u^3(x,t) + \gamma u(x,t) u_x^2(x,t)\right) dx. \end{cases}$$

Actually, the local well-posedness was proved for both periodic and nonperiodic case in the above paper.
The maximum value of T in Theorem 2.1 is called the lifespan of the solution, in general. If $T < \infty$, that is $\limsup_{t\uparrow T} \|u(.,t)\|_{H^s} = \infty$, we say that the solution blows up in finite time. The following theorem tells us that the solution blows up if and only if the first-order derivative blows up.

Theorem 2.2 [13, 41] *Let $u_0(x) \in H^s(\mathbb{S})$, $s > 3/2$, and u be the corresponding solution to problem (1.1) with lifespan T. Then*

$$\sup_{x\in\mathbb{S}, 0\le t<T} |u(x,t)| \le C(\|u_0\|_{H^1}). \tag{2.1}$$

T is bounded if and only if

$$\liminf_{t\uparrow T} \inf_{x\in\mathbb{S}} \{\gamma u_x(x,t)\} = -\infty. \tag{2.2}$$

For $\gamma \neq 0$, we set

$$m(t) := \inf_{x\in\mathbb{S}} \left(u_x(x,t) sign\{\gamma\}\right), \quad t \ge 0, \tag{2.3}$$

where $sign\{a\}$ is the sign function of $a \in \mathbb{R}$ and we set $m_0 := m(t=0)$. Then for every $t \in [0,T)$ there exists at least one point $\xi(t) \in \mathbb{S}$ with $m(t) = u_x(\xi(t),t)$.

Lemma 2.3 [13] *Let $u(t)$ be the solution to (1.1) on $[0,T)$ with initial data $u_0 \in H^s(\mathbb{S})$, $s > 3/2$, as given by Theorem 2.1. Then the function $m(t)$ is almost everywhere differentiable on $[0,T)$, with*

$$\frac{dm(t)}{dt} = u_{tx}(\xi(t),t), \quad a.e. \ on \ (0,T).$$

Consideration of the quantity $m(t)$ for wave breaking comes from an idea of Seliger [34] originally. The rigorous regularity proof is given in [8] for the Camassa-Holm equation.
Set $Q^s = (1-\partial_x^2)^{s/2}$, then the operator Q^{-2} can be expressed by

$$Q^{-2} f = G * f = \int_{\mathbb{T}} G(x-y) f(y) dy$$

for any $f \in L^2(\mathbb{S})$ with

$$G(x) = \frac{\cosh(x - [x] - 1/2)}{2\sinh(1/2)}, \tag{2.4}$$

where $[x]$ denotes the integer part of x. Then equation (1.1) can be rewritten as

$$u_t + \gamma u u_x + \partial_x Q^{-2}\left(\frac{3-\gamma}{2}u^2 + \frac{\gamma}{2}u_x^2\right) = 0. \tag{2.5}$$

Just as in [13, 41], it is easy to derive a equation for $m(t)$ from (2.5) as

$$\frac{dm}{dt} = -\frac{\gamma}{2}m^2 + \frac{3-\gamma}{2}u^2(\xi(t),t) - \left[G * \left(\frac{3-\gamma}{2}u^2 + \frac{\gamma}{2}u_x^2\right)\right](\xi(t),t) \tag{2.6}$$

a.e. on $(0,T)$, where $m(t)$ and $\xi(t)$ are defined in (2.3) and Lemma 2.3.
If $\gamma = 3$, it turns out that (2.6) is a Riccati type equation with negative initial data for any nonconstant u_0. So the solutions to (1.1) in periodic case definitely blow up in finite time with arbitrary nonconstant initial data u_0.
In what follows, we assume that $0 < \gamma < 3$.

3 The best constant for a convolution problem-formulation

To prove the blow-up result, one of the basic ingredients is to analyze equation (2.6). It is clear that the difficult part is the convolution term.
In this section, we consider the following convolution problem

$$G * \left(f^2 + \frac{\alpha}{2}f_x^2\right)(x),$$

where G, defined by (2.4), is the Green function for Q^{-2} in the unit circle, $\alpha > 0$ is a constant, and function f belongs to $H^1(\mathbb{S})$.
Direct computation which already done in [43] yields

$$G * (f^2 + \frac{1}{2}f_x^2)(x) \geq \frac{1}{2}f^2(x),$$

for any $x \in \mathbb{S}$.
Therefore,

$$G * \left(f^2 + \frac{\alpha}{2}f_x^2\right)(x) \geq \min\{\alpha, 1\} G * (f^2 + \frac{1}{2}f_x^2)(x) \geq \min\{\alpha, 1\}\frac{1}{2}f^2(x).$$

Our goal is to find an optimal constant $C(\alpha)$ for the following inequality:

$$G * \left(f^2 + \frac{\alpha}{2}f_x^2\right)(x) \geq C(\alpha) f^2(x), \tag{3.1}$$

for all $f \in H^1(\mathbb{S})$.

For this purpose, let

$$\mathcal{A} = \{f \in H^1(\mathbb{S}) \mid \|f\|_{L^\infty} = 1\}$$

and

$$I[f](x) = G * \left(f^2 + \frac{\alpha}{2} f_x^2\right)(x) = \int_{\mathbb{S}} G(x-y)\left(f^2(y) + \frac{\alpha}{2} f_x^2(y)\right) dy.$$

Since $I[f]$ is a translation invariant on the unit circle $\mathbb{S}$, we can assume that $\mathcal{A}$ is defined on the interval $[0,1]$ with $f \geq 0$ and $f(0) = f(1) = 1$ without loss of generality. Hence finding the best constant for the problem (3.1) is equivalent to finding the minimum value for

$$I[f](0) = \frac{1}{2\sinh(1/2)} \int_0^1 \cosh(x - 1/2)\left(f^2(x) + \frac{\alpha}{2} f_x^2(x)\right) dx.$$

From now on, we follow the variational method discussed in a comprehensive book written by Struwe [36].

It is clear that

$$\begin{aligned} \min\{\alpha, 1\} \frac{1}{2\sinh(1/2)} \int_0^1 \left(f^2(x) + f_x^2(x)\right) dx &\leq I[f](0) \\ \leq \quad \max\{\alpha, 1\} \frac{\cosh(1/2)}{2\sinh(1/2)} \int_0^1 \left(f^2(x) + f_x^2(x)\right) dx, \end{aligned}$$

for any $f \in \mathcal{A}$. The above inequality means that $I[f](0)$ is equivalent to the H^1-norm of f.

Suppose that $\{f_k\}_{k=1}^\infty$ is a minimizing sequence, i.e., $I[f_k](0) \to \inf_{f\in\mathcal{A}} I[f](0)$, as $k \to \infty$. Hence it is easy to show that there exists a subsequence $\{f_{kj}\}_{j=1}^\infty \subset \{f_k\}_{k=1}^\infty$, denoted it by $\{f_k\}_{k=1}^\infty$ also, and a function $g \in \mathcal{A}$ with $f_k \to g$ as $k \to \infty$. For the details we refer to [38].

Due to the identities $\cosh(3x) = \cosh^3(x) + 3\cosh(x)\sinh^2(x)$ and $\sinh(3x) = 4\sinh^3(x) + 3\sinh(x)$, we have

$$\begin{aligned} & I\left[\cosh(x-1/2)/\cosh(1/2)\right](0) \\ = \quad & \frac{1}{2\sinh(1/2)\cosh^2(1/2)} \\ & \times \int_0^1 \left(\cosh^3(x-1/2) + \frac{\alpha}{2}\cosh(x-1/2)\sinh^2(x-1/2)\right) dx \\ = \quad & \frac{1}{2\sinh(1/2)\cosh^2(1/2)} \int_{-1/2}^{1/2} \left(\cosh(3x) + \left(\frac{\alpha}{2} - 3\right)\cosh(x)\sinh^2(x)\right) dx \\ = \quad & \frac{2\sinh(3/2) + (\alpha-6)\sinh^3(1/2)}{6\sinh(1/2)\cosh^2(1/2)} = \frac{6 + (\alpha+2)\sinh^2(1/2)}{6\cosh^2(1/2)} \\ = \quad & 1 - \frac{(4-\alpha)\sinh^2(1/2)}{6\cosh^2(1/2)} < 1 = I[1](0), \end{aligned}$$

provided that $\alpha < 4$.
For the case $\alpha \geq 4$, we consider the family

$$\frac{\beta + \cosh(x - 1/2)}{\beta + \cosh(1/2)},$$

where $\beta > 0$ is a constant to be determined later. By the same steps, one can get

$$\begin{aligned} & I\left[\frac{\beta + \cosh(x - 1/2)}{\beta + \cosh(1/2)}\right](0) \\ = & \frac{6(\beta+1)\sinh(1/2) + (\alpha+2)\sinh^3(1/2) + 6\beta\cosh(1/2)\sinh(1/2) + 3\beta}{6\sinh(1/2)(\beta + \cosh(1/2))^2}. \end{aligned}$$

Direct computation yields

$$I\left[\frac{\beta + \cosh(x - 1/2)}{\beta + \cosh(1/2)}\right](0) < 1,$$

provided that

$$\frac{6\beta(\beta - 1)}{\sinh^2(1/2)} > \alpha - 4.$$

The above inequality implies that 1 is not the minimizer for $I[f](0)$, in other words, there exists region U where the value of g is strictly less than 1.
Let ϕ be a smooth function with compact support in U. One can choose ϵ is sufficient small such that $g + \epsilon\phi \in \mathcal{A}$. Now we set

$$i(t) = I[g + t\epsilon\phi](0) = \int_0^1 G(x)\left((g + t\epsilon\phi)^2 + \frac{\alpha}{2}(g_x + t\epsilon\phi_x)^2\right) dx,$$

where $t \in \mathbb{R}$ such that $g + t\epsilon\phi \in \mathcal{A}$. Since g is the minimizer, we have

$$0 = i'(0) = \epsilon \int_0^1 (2Gg\phi + \alpha G g_x \phi_x) dx = \epsilon \int_0^1 (2Gg - \alpha(Gg_x)_x)\phi dx.$$

Therefore the equation for g in the region $g < 1$ reads

$$\alpha(Gg_x)_x = 2Gg, \text{ with } G(x) = \frac{\cosh(x - 1/2)}{2\sinh(1/2)}.$$

Just as what was done in [38], we have the following claim that $g < 1$ at all points except 0 and 1. So the equation for g is

$$\alpha(Gg_x)_x = 2Gg, \text{ in } (0,1), \text{ with } g(0) = g(1) = 1. \tag{3.2}$$

After changing variable we can rewrite (3.2) as

$$\cosh(x)g''(x) + \sinh(x)g'(x) - \frac{2}{\alpha}\cosh(x)g(x) = 0, \tag{3.3}$$

$x \in (-1/2, 1/2)$, where prime means taking derivative with respect to x.
If $\alpha = 1$, equation (3.3) has been solved in [43] as

$$g = \frac{1 + \arctan(\sinh(x - 1/2))\sinh(x - 1/2)}{1 + \arctan(\sinh(1/2))\sinh(1/2)}, \tag{3.4}$$

for $x \in [0, 1]$.
For general case $\alpha \neq 1$, we will solve the equation in the next section.
However, here we can find the optimal constant for the functional I achieved by g satisfying the equation (3.3). Actually, from the equation (3.2), one has

$$Gg^2 + \frac{\alpha}{2} Gg_x^2 = \frac{\alpha}{2}(Ggg_x)_x .$$

Therefore,

$$\begin{aligned} I[g](0) &= \int_0^1 \frac{\alpha}{2}(Ggg_x)_x \\ &= \frac{\alpha}{2\tanh(1/2)}\left(g(1/2)g'(1/2-0) - g(-1/2)g'(-1/2+0)\right) \\ &= \frac{\alpha}{\tanh(1/2)} g'(1/2-0), \end{aligned}$$

since $g(x)$ is an even function on $[-1/2, 1/2]$, and $g(-1/2) = g(1/2) = 1$.
Hence, we have the following theorem

Theorem 3.1 *For all $f \in H^1(\mathbb{S})$, and $\alpha > 0$, the following inequality holds*

$$G * \left(f^2 + \frac{\alpha}{2} f_x^2\right)(x) \geq C(\alpha) f^2(x), \tag{3.5}$$

with

$$C(\alpha) = \frac{\alpha}{\tanh(1/2)} g'(1/2-0), \tag{3.6}$$

where $g(x)$ is an even function on $[-1/2, 1/2]$ satisfying (3.3).

$$C(1) = \frac{1}{2} + \frac{\arctan(\sinh(1/2))}{2\sinh(1/2) + 2\arctan(\sinh(1/2))\sinh^2(1/2)} \approx 0.869,$$

which has been founded in [43].

Remark 3.1 *From the above variational approach, it implies that $C(\alpha) < 1$ for any $\alpha > 0$.*

4 Solve the ordinary differential equation

For our convenience, we rewrite the equation (3.3) as

$$\cosh(x)u_\lambda''(x) + \sinh(x)u_\lambda'(x) - \lambda(\lambda+1)\cosh(x)u_\lambda(x) = 0, \tag{4.1}$$

$x \in (-1/2, 1/2)$, with $\lambda = \frac{\sqrt{\alpha+8}-\sqrt{\alpha}}{2\sqrt{\alpha}} > 0$.
Now, letting $s = \sinh(x)$ and $v_\lambda(s) = u_\lambda(x)$, then (4.1) changes to

$$(1+s^2)v_\lambda''(s) + 2sv_\lambda'(s) - \lambda(\lambda+1)v_\lambda(s) = 0. \tag{4.2}$$

In general, the solution to (4.2) can be represented as the following power series:

$$v_\lambda(s) = 1 + \sum_{n=1}^{\infty} \frac{\prod_{k=0}^{n-1}(\lambda-2k)(\lambda+1+2k)}{(2n)!} s^{2n}, \tag{4.3}$$

with convergence radius of 1. Hence it is convergent at $s = \sinh(1/2)$.
It is easy to find that, (4.3) is a polynomial with finite terms for λ being a positive even number, i.e., $\lambda = 2m$, $k \in \mathbb{N}$. For $\lambda = 2m+1$, the solution to (4.2) can be obtained by

$$v_\lambda(s) = -v_1(s) \int_0^s \frac{d\tau}{v_1^2(\tau)(1+\tau^2)}, \tag{4.4}$$

where

$$v_1(s) = s\left(1 + \sum_{n=1}^{\infty} \frac{\prod_{k=1}^{n}(\lambda+2k)(\lambda+1-2k)}{(2n+1)!} s^{2n}\right)$$

is another solution to (4.2), which is independent of (4.3).
Due to the strategic steps established here, we can write down the solutions to (4.2) for $\lambda \in \mathbb{N}$. For example, we have

$$u_1(x) = -s\int_0^s \frac{d\tau}{\tau^2(1+\tau^2)} = 1 + s\arctan s = 1 + \sinh(x)\arctan(\sinh(x)),$$

(3.4) is recovered again. We also can write down the following solutions.

$$u_2(x) = 1 + 3s^2 = 1 + 3\sinh^2(x),$$

$$\begin{aligned} u_3(x) &= -s\left(1+\frac{5}{3}s^2\right)\int_0^s \frac{d\tau}{\tau^2\left(1+\frac{5}{3}\tau^2\right)^2(1+\tau^2)} \\ &= 1 + \frac{15}{4}s^2 + s\left(\frac{9}{4}+\frac{15}{4}s^2\right)\arctan s \\ &= 1 + \frac{15}{4}\sinh(x)^2 + s\left(\frac{9}{4}+\frac{15}{4}\sinh(x)^2\right)\arctan\left(\sinh(x)\right), \end{aligned}$$

$$u_4(x) = 1 + 10s^2 + \frac{35}{3}s^4 = 1 + 10\sinh^2(x) + \frac{35}{3}\sinh^4(x),$$

$$\begin{aligned} u_5(x) &= 1 + \frac{105}{64}s^2(7+9s^2) + \frac{15}{64}s(15+70s^2+63s^4)\arctan s \\ &= 1 + \frac{105}{64}\sinh^2(x)\left(7+9\sinh^2(x)\right) \\ &\quad + \frac{15}{64}\sinh(x)\left(15+70\sinh^2(x)+63\sinh^4(x)\right)\arctan\left(\sinh(x)\right), \end{aligned}$$

$$\begin{aligned} u_6(x) &= 1 + 21s^2 + 63s^4 + \frac{231}{5}s^6 \\ &= 1 + 21\sinh^2(x) + 63\sinh^4(x) + \frac{231}{5}\sinh^6(x). \end{aligned}$$

For general $\lambda > 0$, we only have the form of (4.2) at present. We will do some computation in section 6.

5 Blow-up criteria

After local well-posedness of strong solutions (see Theorem 2.1) is established, the next question is whether this local solution can exist globally. As far as we know, the only available global existence result is for the case $\gamma = 1$: see the paper by Constantin [5] for a PDE approach, and the paper by Constantin and McKean [11] for an approach based on the integrable structure of the equation. If the solution exists only for finite time, how about the behavior of the solution when it blows up? What induces the blow-up? On the other hand, to find sufficient conditions to guarantee the finite time blow-up or global existence is of great interest, especially for sufficient conditions added on the initial data.
The main theorem of this section is as following:

Theorem 5.1 *Let $0 < \gamma < 3$. Assume that $u_0 \in H^2(\mathbb{S})$ satisfies $m_0 < 0$ and*

$$m_0^2 > \frac{3-\gamma}{2\gamma}\left(1 - C\left(\frac{2\gamma}{3-\gamma}\right)\right)\frac{\cosh(1/2)}{\sinh(1/2)}\|u_0\|^2_{H^1(\mathbb{S})}, \tag{5.1}$$

where $C\left(\frac{2\gamma}{3-\gamma}\right)$ is defined by (3.6). Then the life span $T > 0$ of the corresponding solution to (1.1) is finite.

Remark 5.1 *When $\gamma = 1$, we recover the theorem established in [43]. The cases for $\gamma < 0$ and $\gamma > 3$ were discussed in [41, 42].*

First, we have the following blow-up result for a Riccati type ordinary differential equation.

Lemma 5.2 [43] *Assume that a differentiable function $y(t)$ satisfies*

$$y'(t) \leq -Cy^2(t) + K, \tag{5.2}$$

with constants $C, K > 0$. If the initial datum $y(0) = y_0 < -\sqrt{\frac{K}{C}}$, then the solution to (5.2) goes to $-\infty$ in finite time.

Secondly, let us recall the best constant for a Sobolev inequality proved in [38].

$$\|f\|^2_{L^\infty(\mathbb{S})} \leq \frac{\cosh(1/2)}{2\sinh(1/2)} \|f\|^2_{H^1(\mathbb{S})}, \tag{5.3}$$

for $f \in H^1(\mathbb{S})$. Moreover, it is an optimal constant for the Sobolev imbedding $H^1 \subset L^\infty$ in the sense that (5.3) holds if and only if $f(x) = \lambda G(x-y)$ for some $\lambda, y \in \mathbb{R}$.
We start the proof for the main theorem from (2.6).

$$\begin{aligned}
\frac{dm}{dt} &= -\frac{\gamma}{2}m^2 + \frac{3-\gamma}{2}u^2(\xi(t),t) - \left[G * \left(\frac{3-\gamma}{2}u^2 + \frac{\gamma}{2}u_x^2\right)\right](\xi(t),t) \\
&= -\frac{\gamma}{2}m^2 + \frac{3-\gamma}{2}u^2(\xi(t),t) - \frac{3-\gamma}{2}\left[G * \left(u^2 + \frac{1}{2}\frac{2\gamma}{3-\gamma}u_x^2\right)\right](\xi(t),t) \\
&\leq -\frac{\gamma}{2}m^2 + \frac{3-\gamma}{2}u^2(\xi(t),t) - \frac{3-\gamma}{2}C\left(\frac{2\gamma}{3-\gamma}\right)u^2(\xi(t),t) \\
&\leq -\frac{\gamma}{2}m^2 + \frac{3-\gamma}{2}\left(1 - C\left(\frac{2\gamma}{3-\gamma}\right)\right)u^2(\xi(t),t) \\
&\leq -\frac{\gamma}{2}m^2 + \frac{3-\gamma}{2}\left(1 - C\left(\frac{2\gamma}{3-\gamma}\right)\right)\frac{\cosh(1/2)}{2\sinh(1/2)}\|u_0\|^2_{H^1(\mathbb{S})},
\end{aligned}$$

where we used (3.5) and (5.3).
So, the proof can be completed by using the condition in Theorem 5.1 and Lemma 5.2.

6 Another presentation and numerical simulation

We have the equation (4.2), and the local solution to (4.2) can be represented as the power series (4.4), which is convergent at $s = \sinh(1/2) = 0.521\cdots$.
By the transformation of variables

$$z := -s^2, y_\lambda(s) := v_\lambda(s)$$

and let

$$a := -\lambda/2, b := (\lambda+1)/2, c := 1/2,$$

then

$$v_\lambda(s) = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \prod_{k=0}^{n-1} \frac{(a+k)(b+k)}{c+k} =: F(a,b,c;z), \tag{6.1}$$

where $F(a,b,c;z)$ is called the hypergeometric function, a regular solution of the hypergeometric differential equation

$$z(1-z)y''_\lambda(z) + [c-(a+b+1)z]y'_\lambda(z) - aby_\lambda(z) = 0.$$

Since

$$F'(a,b,c;z) = \frac{ab}{c}F(a+1,b+1,c+1;z),$$

we obtain the analytic expression

$$C(\alpha) = \frac{\cosh^2(1/2)F(a+1,b+1,c+1;-\sinh^2(1/2))}{\sinh(1/2)F(a,b,c;-\sinh^2(1/2))},$$

where $\alpha = 2/(\lambda(\lambda+1))$.

Although the value of $C(\alpha)$ for each λ can be obtained by calling the hypergeometric functions in softwares such as Mathematica, Maple or MATLAB, generally the calculation based on (6.1), thus the calculations are not efficient. In the following, we give an efficient method for calculating $C(\alpha)$.

Define

$$q_\lambda(s) := \frac{v'_\lambda(s)}{\lambda(\lambda+1)v_\lambda(s)}, \quad \lambda > 0,$$

then $q_\lambda(s)$ is the solution of the following initial value problem of the first order ordinary differential equation

$$q'_\lambda(s) + \frac{2s}{1+s^2}q_\lambda(s) + \mu q_\lambda^2(s) = \frac{1}{1+s^2}, \quad q_\lambda(0) = 0, \tag{6.2}$$

where $\mu := \lambda(\lambda+1)$.

Thus

$$C(\alpha) = \frac{\cosh^2(1/2)q_\lambda(\sinh(1/2))}{\sinh(1/2)}. \tag{6.3}$$

By using MATLAB programme, we can plot the graph of $C(\alpha)$ as Fig. 1. Here α is taken from 0.01 to 10 with equal step length 0.01. The detailed MATLAB code is given in the appendix.

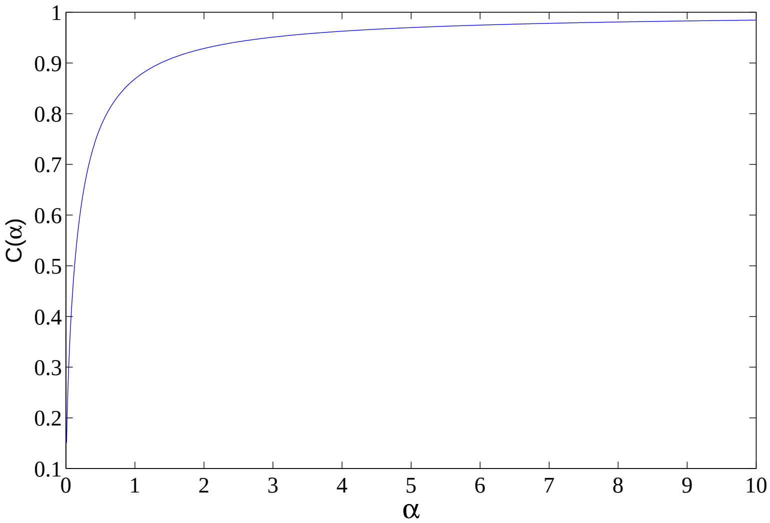

Fig. 1

From Fig. 1 we see that $C(\alpha)$ is a strictly increasing function of α which can be proved analytically as follows.
Differentiate both sides of (6.2) with respect to μ, we have a linear differential equation of $q_{\lambda\mu}(s) = \partial q_\lambda(s)/\partial\mu$:

$$q'_{\lambda\mu}(s) + 2\left(\mu q_\lambda(s) + \frac{s}{1+s^2}\right) q_{\lambda\mu}(s) + q_\lambda^2(s) = 0, \quad q_\lambda(0) = 0. \tag{6.4}$$

The solution to (6.4) is

$$q_{\lambda\mu}(s) = -\frac{1}{1+s^2}\int_0^s (1+\tau^2)\exp\left(-2\mu\int_\tau^s q_\lambda(t)\,\mathrm{d}t\right) q_\lambda^2(\tau)\,\mathrm{d}\tau < 0. \tag{6.5}$$

While

$$q_{\lambda\alpha}(s) = \frac{\partial q_\lambda(s)}{\partial\mu}\frac{\partial\mu}{\partial\alpha} = q_{\lambda\mu}\cdot\frac{-2}{\alpha^2} > 0.$$

This completes the proof due to (6.3).

7 Appendix

Fig. 1 is plotted by two MATLAB routines for calculating $C(\alpha)$. We use MATLAB because of its advantage of efficient vector operations. The argument alpha can be a vector.

1. The main function routine, MATLAB m-file named bestc.m:

   function C=bestc(alpha)

   % Input: alpha, may be a scalar or a vector;

   % Output: C, the best coefficient corresponding to alpha, When alpha is a vector, C is also a vector with the same size as alpha.

   T=.52109530549374738495; % T = sinh(1/2)

   G=2.4401300568286909964; % G = T+Tˆ(-1)

   options=odeset('RelTol',2.221e-14,'ABsTol',1e-15); % Set ODE solver's relative error tolerance and absolute error tolerance.

   [S,Y]=ode45(@rod,[0,T],0*alpha,options,alpha); % Call ODE solver ode45.

   C=Y(end,:)*G;

   % End of the main routine.

2. The ODE-file named rod.m is as follows:

   function dqds = rod(s,q,alpha)

   dqds = (1-2*s*q)/(1+sˆ2)-2*q.ˆ2./alpha;

   % End of the ODE-file.

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Excess Charge for Pseudo-Relativistic Atoms in Hartree-Fock Theory

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Abstract. We prove within the Hartree-Fock theory of pseudo-relativistic atoms that the maximal negative ionization charge and the ionization energy of an atom remain bounded independently of the nuclear charge Z and the fine structure constant α as long as $Z\alpha$ is bounded.

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1 Introduction

A long standing open problem in the mathematical physics literature is the Ionization conjecture. It can be formulated as follows. Consider atoms with arbitrarily large nuclear charge Z, is it true that the radius (see Definition 1.8) and the maximal negative ionization remain bounded? A positive answer to this question in the non-relativistic Hartree-Fock model has been given by the second author in [23]. One of the aims of the present paper is to extend the result taking into account some relativistic effects. The ionization conjecture for the full Schrödinger theory is still open both in the non-relativistic and relativistic case. See [13], [16], [17], [6], [7] and [22] for some Z-dependent bounds on the maximal negative ionization. The best result is that $N(Z) = Z + O(Z^a)$ with $a = 47/56$ where $N(Z)$ denotes the maximal number of electrons a nucleus of charge Z binds (see [6], [7] and [22]) .

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As a model for an atom with nuclear charge Z and N electrons we consider (in units where $\hbar = m = e = 1$) the operator

$$H = \sum_{i=1}^{N} \alpha^{-1}\big(\sqrt{-\Delta_i + \alpha^{-2}} - \alpha^{-1} - \frac{Z\alpha}{|\mathbf{x}_i|}\big) + \sum_{1\le i<j\le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \qquad (1)$$

where α is Sommerfeld's fine structure constant. The operator H acts on a dense subset of the N body Hilbert space $\mathcal{H}_F := \wedge_{i=1}^{N} L^2(\mathbb{R}^3;\mathbb{C}^q)$ of antisymmetric wave functions, where q is the number of spin states. The operator H is bounded from below on this subspace if $Z\alpha \le 2/\pi$ (see [9] for $N = 1$, [5] and [19] for $N \ge 1$). In this paper we will consider the sub-critical case $Z\alpha < 2/\pi$. Let us notice here that to define the operator H there is an issue. Indeed for $Z\alpha < 2/\pi$ the nuclear potential is only a small form perturbation of the kinetic energy and hence one needs to work with forms to define the operator H. This has been done in detail in [2].

The quantum ground state energy is the infimum of the spectrum of H considered as an operator acting on $\mathcal{H}_F$. In the Hartree-Fock approximation one restricts to wave-functions ψ which are pure wedge products, also called Slater determinants:

$$\psi(\mathbf{x}_1,\sigma_1,\mathbf{x}_2,\sigma_2,\dots,\mathbf{x}_N,\sigma_N) = \tfrac{1}{\sqrt{N!}}\det(u_i(\mathbf{x}_j,\sigma_j))_{i,j=1}^{N}, \qquad (2)$$

with $\{u_i\}_{i=1}^{N}$ orthonormal in $L^2(\mathbb{R}^3;\mathbb{C}^q)$. The u_i's are also called orbitals. Notice that $\|\psi\|_{L^2(\mathbb{R}^{3N},\mathbb{C}^{qN})} = 1$. The Hartree-Fock ground state energy is

$$E^{\mathrm{HF}}(N,Z,\alpha) := \inf\{\mathrm{q}(\psi,\psi)|\psi \in \mathcal{Q}(H) \text{ and } \psi \text{ a Slater determinant}\},$$

with $\mathtt{q}$ the quadratic form defined by H and $\mathcal{Q}(H)$ the corresponding form domain.

One of the main result of the paper is the following.

Theorem 1.1. *Let $Z \ge 1$ and $\alpha > 0$. Let $Z\alpha = \kappa$ and assume that $0 \le \kappa < 2/\pi$. There is a constant $Q > 0$ depending only on κ such that if N is such that a Hartree-Fock minimizer exists then $N \le Z + Q$.*[2]

The idea of the proof is the same as in [23]. One shows that the Thomas-Fermi model is a good approximation of the Hartree-Fock model except in the region far away from the nucleus. We first introduce some notation in order to introduce the Hartree-Fock and Thomas-Fermi models.

[2] In order to prove this result we need that $N < CZ$ for a positive constant C. We do not include a proof of this fact here for simplicity and since a much stronger result has been proved by Lieb in [13] for $\alpha Z < 1/2$. The needed extension of this result of Lieb to $\alpha Z < 2/\pi$ will appear in [3] (see Theorem 1.6 below).

1.1 Notation

Let e be the quadratic form with domain $H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$ such that

$$\mathrm{e}(u,v) = (E(\mathbf{p})^{\frac{1}{2}}u, E(\mathbf{p})^{\frac{1}{2}}v) \text{ for all } u,v \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q), \tag{3}$$

where $E(\mathbf{p})$ denotes the operator $E(i\nabla) = \sqrt{-\Delta + \alpha^{-2}}$. As usual (u,v) denotes the scalar product of u and v in $L^2(\mathbb{R}^3, \mathbb{C}^q)$. Let $V(\mathbf{x}) := Z\alpha/|\mathbf{x}|$ and v be the quadratic form with domain $H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$ defined by

$$\mathrm{v}(u,v) = (V^{\frac{1}{2}}u, V^{\frac{1}{2}}v) \text{ for all } u,v \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q). \tag{4}$$

From [10, 5.33 p.307] we have

$$\int_{\mathbb{R}^3} \frac{|f(\mathbf{x})|^2}{|\mathbf{x}|}\, d\mathbf{x} \le \frac{2}{\pi} \int_{\mathbb{R}^3} |\mathbf{p}||\hat{f}(\mathbf{p})|^2 \, d\mathbf{p} \text{ for } f \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}) \tag{5}$$

with $\hat{f}$ the Fourier transform of f. Thus since $Z\alpha \le 2/\pi$ and $E(\mathbf{p}) \ge |\mathbf{p}|$ it follows that $\mathrm{v}(u,u) \le \mathrm{e}(u,u)$ for all $u \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$.
In the following t denotes the quadratic form associated to the kinetic energy; i.e. for all $u,v \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$

$$\mathrm{t}(u,v) := \alpha^{-1}\mathrm{e}(u,v) - \alpha^{-2}(u,v) = \alpha^{-1}(T(\mathbf{p})^{\frac{1}{2}}u, T(\mathbf{p})^{\frac{1}{2}}v), \tag{6}$$

with $T(\mathbf{p}) := E(\mathbf{p}) - \alpha^{-1}$.
A *density matrix* γ is a self-adjoint trace class operator that satisfies the operator inequality $0 \le \gamma \le Id$. A density matrix $\gamma : L^2(\mathbb{R}^3; \mathbb{C}^q) \to L^2(\mathbb{R}^3; \mathbb{C}^q)$ has an integral kernel

$$\gamma\,(\mathbf{x}, \sigma, \mathbf{y}, \tau) = \sum_j \lambda_j u_j(\mathbf{x}, \sigma) u_j(\mathbf{y}, \tau)^*, \tag{7}$$

where λ_j, u_j are the eigenvalues and corresponding eigenfunctions of γ. We choose the u_j's to be orthonormal in $L^2(\mathbb{R}^3, \mathbb{C}^q)$. Let $\rho_\gamma \in L^1(\mathbb{R}^3)$ denote the 1-particle density associated to γ given by

$$\rho_\gamma(\mathbf{x}) = \sum_{\sigma=1}^{q} \sum_j \lambda_j |u_j(\mathbf{x}, \sigma)|^2.$$

We define

$$\mathcal{A} := \{\gamma \text{ density matrix: } \operatorname{Tr}[T(\mathbf{p})\gamma] < +\infty\}, \tag{8}$$

where for $\gamma \in \mathcal{A}$ written as in (7) $\operatorname{Tr}[T(\mathbf{p})\gamma] := \operatorname{Tr}[E(\mathbf{p})\gamma] - \alpha^{-1}\operatorname{Tr}[\gamma]$ and

$$\operatorname{Tr}[E(\mathbf{p})\gamma] := \sum_j \lambda_j \mathrm{e}(u_j, u_j). \tag{9}$$

Similarly we use the following notation $\operatorname{Tr}[V\gamma] := \sum_j \lambda_j \mathrm{v}(u_j, u_j)$.

Remark 1.2. *If $\gamma \in \mathcal{A}$ then $\rho_\gamma \in L^1(\mathbb{R}^3)$ since γ is trace class and $\rho_\gamma \in L^{4/3}(\mathbb{R}^3)$. The second inclusion follows from Daubechies' inequality, a generalization of the Lieb-Thirring inequality (see Theorem 2.3).*

1.2 Hartree-Fock theory

In Hartree-Fock theory one considers wave functions that are pure wedge products and that satisfy the right statistics: determinantal wave functions as in (2). To define the HF-energy functional it is convenient to use the one to one correspondence between Slater determinants and projections onto finite dimensional subspaces of $L^2(\mathbb{R}^3, \mathbb{C}^q)$. Indeed if ψ is given by (2) and γ is the projection onto the space spanned by $u_1, \ldots, u_N$ the energy expectation depends only on γ: $(\psi, H\psi) = \mathcal{E}^{\mathrm{HF}}(\gamma)$. Here $\mathcal{E}^{\mathrm{HF}}$ defines the HF-energy functional

$$\mathcal{E}^{\mathrm{HF}}(\gamma) = \alpha^{-1}\,\mathrm{Tr}[(T(\mathbf{p}) - V)\gamma] + \mathcal{D}(\gamma) - \mathcal{E}x\,(\gamma)\,, \tag{10}$$

where $\mathcal{D}(\gamma)$ is the direct Coulomb energy

$$\mathcal{D}(\gamma) = \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{x})\rho_\gamma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y},$$

and $\mathcal{E}x(\gamma)$ is the exchange Coulomb energy

$$\mathcal{E}x(\gamma) = \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\mathrm{Tr}_{\mathbb{C}^q}\left[|\gamma(\mathbf{x},\mathbf{y})|^2\right]}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y},$$

where we think of the integral kernel $\gamma(x, y)$ as a $q \times q$ matrix.
Using projections we can define as follows the HF-ground state.

Definition 1.3 (The HF-ground state). *Let $Z > 0$ be a real number and $N \geq 0$ be an integer. The HF-ground state energy is*

$$E^{\mathrm{HF}}(N, Z, \alpha) := \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma^2 = \gamma,\ \gamma \in \mathcal{A},\ \ \mathrm{Tr}[\gamma] = N\right\}.$$

If a minimizer exists we say that the atom has a HF ground state described by γ^{HF}.

We may extend the definition of the HF-functional from projections to density matrices in $\mathcal{A}$. We first notice that if $\gamma \in \mathcal{A}$, then all the terms in $\mathcal{E}^{\mathrm{HF}}(\gamma)$ are finite. From (5) it follows that

$$\mathrm{Tr}[V\gamma] = \sum_j \lambda_j \mathrm{v}(u_j, u_j) \leq \sum_j \lambda_j \mathrm{e}(u_j, u_j) = \mathrm{Tr}[E(\mathbf{p})\gamma].$$

On the other hand if $\gamma \in \mathcal{A}$ then $\rho_\gamma \in L^1(\mathbb{R}^3) \cap L^{\frac{4}{3}}(\mathbb{R}^3)$ (see Remark 1.2). By Hölder's inequality $\rho_\gamma \in L^{\frac{6}{5}}(\mathbb{R}^3)$ and hence $\mathcal{D}(\gamma)$ is bounded by Hardy-Littlewood-Sobolev's inequality. The boundness of the exchange term follows from $0 \leq \mathcal{E}x(\gamma) \leq \mathcal{D}(\gamma)$. On the other hand if γ is a density matrix with $\gamma \notin \mathcal{A}$ then $\mathcal{E}^{\mathrm{HF}}(\gamma) = \infty$. Here we use also that $Z\alpha < 2/\pi$.
Extending the set where we minimize, we could have lowered the ground state energy and/or changed the minimizer. That this is not the case follows from Lieb's variational principle.

Theorem 1.4 (Lieb's variational principle, [12]). *For all N non-negative integers it holds that*

$$\inf\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma \in \mathcal{A},\ \gamma^2 = \gamma,\ \mathrm{Tr}[\gamma] = N\} = \inf\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma \in \mathcal{A},\ \mathrm{Tr}[\gamma] = N\},$$

and if the infimum over all density matrices is attained so is the infimum over projections.

The following existence theorem for the HF-minimizer in the pseudo-relativistic case has been recently proved in [2].

Theorem 1.5. *Let $Z\alpha < 2/\pi$ and let $N \geq 2$ be a positive integer such that $N < Z + 1$.*
Then there exists an N-dimensional projection $\gamma^{\mathrm{HF}} = \gamma^{\mathrm{HF}}(N, Z, \alpha)$ minimizing the HF-energy functional $\mathcal{E}^{\mathrm{HF}}$ given by (10), that is, $E^{\mathrm{HF}}(N, Z, \alpha)$ is attained. Moreover, one can write

$$\gamma^{\mathrm{HF}}(\mathbf{x}, \sigma, \mathbf{y}, \tau) = \sum_{i=1}^{N} u_i(\mathbf{x}, \sigma) u_i(\mathbf{y}, \tau)^*,$$

with $u_i \in L^2(\mathbb{R}^3, \mathbb{C}^q)$, $i = 1, \ldots, N$, orthonormal, such that the HF-orbitals $\{u_i\}_{i=1}^N$ satisfy:

1. *$h_{\gamma^{\mathrm{HF}}} u_i = \varepsilon_i u_i$, with $0 > \varepsilon_N \geq \varepsilon_{N-1} \geq \cdots \geq \varepsilon_1 > -\alpha^{-1}$ and*

$$h_{\gamma^{\mathrm{HF}}} := T(\mathbf{p}) - \frac{Z\alpha}{|\mathbf{x}|} + \rho^{\mathrm{HF}} * |\mathbf{x}|^{-1} - \mathcal{K}_{\gamma^{\mathrm{HF}}}, \tag{11}$$

where ρ^{HF} denotes the density of the HF-minimizer and for $f \in H^{\frac{1}{2}}(\mathbb{R}^3)$

$$(\mathcal{K}_{\gamma^{\mathrm{HF}}} f)(\mathbf{x}, \sigma) = \sum_{i=1}^{N} u_i(\mathbf{x}, \sigma) \sum_{\tau=1}^{q} \int_{\mathbb{R}^3} u_i(\mathbf{y}, \tau)^* f(\mathbf{y}, \tau) |\mathbf{x} - \mathbf{y}|^{-1} d\mathbf{y}.$$

2. *$u_i \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^q)$ for $i = 1, \ldots, N$;*
3. *$u_i \in H^1(\mathbb{R}^3 \setminus B_R(0))$ for all $R > 0$ and $i = 1, \ldots, N$.*

In the opposite direction the following result gives an upper bound on the excess charge.

Theorem 1.6. *Let $\alpha Z < \frac{2}{\pi}$. If N is a positive integer such that $N > 2Z + 1$ there are no minimizers for the HF-energy functional.*

This theorem for $Z\alpha < 1/2$ was proved by Lieb in [13]. With an improved approximation argument the proof can be extended to $Z\alpha < 2/\pi$ (see [3]). Notice that both proofs work not only in the Hartree-Fock approximation but for the minimization problem on $\wedge^N L^2(\mathbb{R}^3)$.

Definition 1.7. *Let γ^{HF} be the HF-minimizer. The function*

$$\varphi^{\mathrm{HF}}(\mathbf{x}) := \frac{Z}{|\mathbf{x}|} - \int_{\mathbb{R}^3} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \text{ for } \mathbf{x} \in \mathbb{R}^3,$$

is called the HF-mean field potential and

$$\Phi_R^{\mathrm{HF}}(\mathbf{x}) := \frac{Z}{|\mathbf{x}|} - \int_{|\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \text{ for } \mathbf{x} \in \mathbb{R}^3,$$

is the HF-screened nuclear potential.

Definition 1.8. *We define the HF-radius $R_{Z,N}^{\mathrm{HF}}(\nu)$ to the ν last electrons by*

$$\int_{|\mathbf{x}| \geq R_{Z,N}^{\mathrm{HF}}(\nu)} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} = \nu.$$

1.3 A bit of Thomas-Fermi theory

In this subsection we present briefly the Thomas-Fermi theory and especially the result that will be used in the rest of the paper. We refer the interested reader to [11].

Let U be a potential in $L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with

$$\inf\{\|W\|_\infty : U - W \in L^{\frac{5}{2}}(\mathbb{R}^3)\} = 0.$$

Then the TF-energy functional is defined by

$$\mathcal{E}_U^{\mathrm{TF}}(\rho) = \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}} \int_{\mathbb{R}^3} \rho(\mathbf{x})^{\frac{5}{3}} d\mathbf{x} - \int_{\mathbb{R}^3} U(\mathbf{x})\rho(\mathbf{x}) d\mathbf{x} + \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y},$$

on non-negative functions $\rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$. As before, q denotes the number of spin states.

We recall some properties of the TF-model, see [18].

Theorem 1.9. *Let U be as above. For all $N' \geq 0$ there exists a unique non-negative $\rho_U^{\mathrm{TF}} \in L^{5/3}(\mathbb{R}^3)$ such that $\int \rho_U^{\mathrm{TF}} \leq N'$ and*

$$\mathcal{E}_U^{\mathrm{TF}}(\rho_V^{\mathrm{TF}}) = \inf\{\mathcal{E}_U^{\mathrm{TF}}(\rho) : \rho \in L^{5/3}(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \rho(\mathbf{x})\, d\mathbf{x} \leq N'\}.$$

There exists a unique chemical potential $\mu_U^{\mathrm{TF}}(N')$, with $0 \leq \mu_U^{\mathrm{TF}}(N') \leq \sup U$, such that ρ_U^{TF} is uniquely characterized by

$$\begin{aligned} &\mathcal{E}_U^{\mathrm{TF}}(\rho_U^{\mathrm{TF}}) + \mu_U^{\mathrm{TF}}(N') \int_{\mathbb{R}^3} \rho_U^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} \\ = \ &\inf\{\mathcal{E}_U^{\mathrm{TF}}(\rho) + \mu_U^{\mathrm{TF}}(N') \int_{\mathbb{R}^3} \rho(\mathbf{x})\, d\mathbf{x} : 0 \leq \rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)\}. \end{aligned}$$

Moreover ρ_U^{TF} is the unique solution in $L^{5/3}(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$ to the TF-equation

$$\tfrac{1}{2}(\tfrac{6\pi^2}{q})^{\frac{2}{3}}(\rho_U^{\mathrm{TF}}(\mathbf{x}))^{\frac{2}{3}} = \left[U(\mathbf{x}) - \rho_U^{\mathrm{TF}} * |\mathbf{x}|^{-1} - \mu_U^{\mathrm{TF}}(N')\right]_+ .$$

If $\mu_U^{\mathrm{TF}}(N') > 0$ then $\int \rho_U^{\mathrm{TF}} = N'$. For all $\mu > 0$ there is a unique minimizer $0 \le \rho \in L^{5/3}(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$ to $\mathcal{E}_U^{\mathrm{TF}}(\rho) + \mu\int\rho$.

One defines the *TF-mean field potential* φ_U^{TF}, the *TF-screened nuclear potential* $\Phi_{U,R}^{\mathrm{TF}}$ and the TF-radius $R_{N,Z}^{\mathrm{TF}}(\nu)$ to the ν last-electron similarly as in Definitions 1.7 and 1.8 replacing the HF-density with the TF-density.

THEOREM 1.10. *If $U(\mathbf{x}) = Z/|\mathbf{x}|$ (the Coulomb potential), then the minimizer of $\mathcal{E}_U^{\mathrm{TF}}$, under the condition $\int\rho \le N$, exists for every N. Moreover, $\mu_U^{\mathrm{TF}}(N) = 0$ if and only if $N \ge Z$.*

When $U(\mathbf{x}) = Z/|\mathbf{x}|$ we denote the minimizer of the TF-functional, under the condition $\int\rho\le Z$, simply by ρ^{TF} and $\int\rho^{\mathrm{TF}} = Z$. Correspondingly φ^{TF} and Φ_R^{TF} denote, respectively, its mean field and screened nuclear potential. With this notation

$$\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = -e_0 Z^{\frac{7}{3}}, \tag{12}$$

where e_0 is the total binding energy of a neutral TF-atom of unit nuclear charge. We recall here a result due to Sommerfeld on the asymptotic behavior of the TF-mean field potential, see [23, Th. 4.6].

THEOREM 1.11 (Sommerfeld asymptotics). *Assume that the potential U is continuous and harmonic for $|\mathbf{x}| > R$ and that it satisfies $\lim_{|\mathbf{x}|\to\infty} U(\mathbf{x}) = 0$. Consider the corresponding TF-mean field potential φ_U^{TF} and assume that $\mu_U^{\mathrm{TF}} < \liminf_{r\searrow R}\inf_{|\mathbf{x}|=r}\varphi_U^{\mathrm{TF}}(\mathbf{x})$. With $\zeta = (-7+\sqrt{73})/2$ define*

$$\begin{aligned} a(R) &:= \liminf_{r\searrow R}\sup_{|\mathbf{x}|=r}\Big[\Big(\frac{\varphi_U^{\mathrm{TF}}(\mathbf{x})}{3^4 2^{-1}q^{-2}\pi^2 r^{-4}}\Big)^{-\frac{1}{2}} - 1\Big]r^{\zeta} \\ A(R,\mu_U^{\mathrm{TF}}) &:= \liminf_{r\searrow R}\sup_{|\mathbf{x}|=r}\Big[\frac{\varphi_U^{\mathrm{TF}}(\mathbf{x}) - \mu_U^{\mathrm{TF}}}{3^4 2^{-1}q^{-2}\pi^2 r^{-4}} - 1\Big]r^{\zeta}. \end{aligned}$$

Then we find for all $|\mathbf{x}| > R$

$$\begin{aligned} \varphi_U^{\mathrm{TF}}(\mathbf{x}) &\le \tfrac{3^4\pi^2}{2q^2}(1 + A(R,\mu_U^{\mathrm{TF}})|\mathbf{x}|^{-\zeta})|\mathbf{x}|^{-4} + \mu_U^{\mathrm{TF}} \quad \textit{and} \\ \varphi_U^{\mathrm{TF}}(\mathbf{x}) &\ge \max\Big\{\tfrac{3^4\pi^2}{2q^2}(1 + a(R)|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-4}, \nu(\mu_U^{\mathrm{TF}})|\mathbf{x}|^{-1}\Big\}, \end{aligned}$$

where

$$\nu(\mu_U^{\mathrm{TF}}) := \inf_{|\mathbf{x}|\ge R}\max\big\{\tfrac{3^4\pi^2}{2q^2}(1 + a(R)|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-3}, \mu_U^{\mathrm{TF}}|\mathbf{x}|\big\}.$$

For easy reference we give here the estimate on the TF-mean field potential corresponding to the Coulomb potential.

THEOREM 1.12 (Atomic Sommerfeld estimate, [23, Thm 5.2-5.4]). *The atomic TF-mean field potential satisfies the bound*

$$\frac{Z}{|\mathbf{x}|} - \min\left\{\frac{Z}{|\mathbf{x}|}, \frac{Z^{\frac{4}{3}}}{2\beta_0}\right\} \leq \varphi^{\mathrm{TF}}(\mathbf{x}) \leq \min\left\{\tfrac{3^4\pi^2}{2q^2}\frac{1}{|\mathbf{x}|^4}, \frac{Z}{|\mathbf{x}|}\right\}, \tag{13}$$

with $2\beta_0 = \pi^{\frac{2}{3}}3^{-\frac{5}{3}}2^{-\frac{1}{3}}q^{-\frac{2}{3}}$, *and for* $|\mathbf{x}| \geq R > 0$

$$\varphi^{\mathrm{TF}}(\mathbf{x}) \geq \tfrac{3^4\pi^2}{2q^2}(1 + a(R)|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-4},$$

where ζ *and* $a(R)$ *are defined in Theorem 1.11.*

COROLLARY 1.13. *Let* ζ *and* β_0 *be defined as in Theorem 1.11 and 1.12 respectively. Then the TF-mean field potential satisfies the bound*

$$\varphi^{\mathrm{TF}}(\mathbf{x}) \geq \begin{cases} \dfrac{Z}{|\mathbf{x}|} - \dfrac{Z^{\frac{4}{3}}}{2\beta_0} & \text{if } |\mathbf{x}| \leq \beta_0 Z^{-\frac{1}{3}} \\ \dfrac{3^4\pi^2}{2q^2}(1 + aZ^{-\frac{\zeta}{3}}|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-4} & \text{if } |\mathbf{x}| > \beta_0 Z^{-\frac{1}{3}}, \end{cases}$$

with $a = \beta_0^{\zeta}(3^2\pi/(q\beta_0^{\frac{3}{2}}) - 1)$.

COROLLARY 1.14. *The TF-screened nuclear potential satisfies*

$$\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) \leq \tfrac{3^4 2\pi^2}{q^2}|\mathbf{x}|^{-4} \quad \text{for all } \mathbf{x} \in \mathbb{R}^3.$$

COROLLARY 1.15. *The following estimate holds*

$$\int_{\mathbb{R}^3} (\rho^{\mathrm{TF}}(\mathbf{x}))^{\frac{5}{3}} d\mathbf{x} \leq 4\tfrac{2^{\frac{2}{3}}}{\pi^2}\tfrac{5}{7}q^{\frac{4}{3}}Z^{\frac{7}{3}}.$$

Proof. By the TF-equation and since $\mu^{\mathrm{TF}} = 0$ we find

$$\int_{\mathbb{R}^3} (\rho^{\mathrm{TF}}(\mathbf{x}))^{\frac{5}{3}} d\mathbf{x} = 2^{\frac{5}{2}}(\tfrac{q}{6\pi^2})^{\frac{5}{3}} \int_{\mathbb{R}^3} (\varphi^{\mathrm{TF}}(\mathbf{x}))^{\frac{5}{2}} d\mathbf{x}.$$

The estimate follows from the atomic Sommerfeld upper bound. □

1.4 Construction and main results

We present the basic idea for the proof of Theorem 1.1. Let us consider an atomic system with $N \geq 2$ fermionic particles and a nucleus of charge $Z \geq 1$ with $Z\alpha = \kappa$ and $0 \leq \kappa < 2/\pi$. We assume that $N \geq Z$ and that N is such that a HF-minimizer exists. That is: there exists a density matrix $\gamma^{\mathrm{HF}} \in \mathcal{A}$ such that $\mathrm{Tr}[\gamma^{\mathrm{HF}}] = N$ and

$$\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma = \gamma^*, 0 \leq \gamma \leq I, \mathrm{Tr}[\gamma] = N\right\}.$$

Let ρ^{TF} be the TF-minimizer with potential $U(\mathbf{x}) = Z/|\mathbf{x}|$ and under the condition $\int \rho^{\mathrm{TF}} = Z$. We know that such a minimizer exists and that the corresponding chemical potential is zero (see Theorem 1.10).
Denoting by ρ^{HF} the density of the minimizer γ^{HF}, we find for all $r > 0$

$$\begin{aligned} N &= \int_{\mathbb{R}^3} \rho^{\mathrm{HF}}(\mathbf{x}) d\mathbf{x} \\ &= \int_{|\mathbf{x}|<r} \left[\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})\right] d\mathbf{x} + \int_{|\mathbf{x}|<r} \rho^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} + \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x}. \end{aligned}$$

By the equalities above and since $\int_{|\mathbf{x}|<r} \rho^{\mathrm{TF}}(\mathbf{x}) d\mathbf{x} \leq Z$, Theorem 1.1 follows from the following result.

Theorem 1.16. *There exist $r > 0$ and positive constants c_1 and c_2 independent of N and Z but possibly depending on κ such that*

$$\int_{|\mathbf{x}|<r} \left[\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})\right] d\mathbf{x} \leq c_1 \text{ and } \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x}) d\mathbf{x} \leq c_2.$$

The following theorem is the principal ingredient in the proof of the previous one and is the main technical estimate in the paper.

Theorem 1.17. *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. Assume $N \geq Z \geq 1$.*
Then there exist universal constants $\alpha_0 > 0$, $0 < \varepsilon < 4$ and C_M and C_Φ depending on κ such that for all $\alpha \leq \alpha_0$

$$\left|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})\right| \leq C_\Phi |\mathbf{x}|^{-4+\varepsilon} + C_M.$$

This main estimate is proven by an iterative procedure. We first prove the estimate for small $\mathbf{x}$ (i.e. $|\mathbf{x}| \leq \beta_0 Z^{-\frac{1}{3}}$), then for intermediate $\mathbf{x}$ (i.e. up to a fixed distance independent of Z) and finally for big $\mathbf{x}$.
By proving Theorem 1.17 we also get the following interesting results. The proofs of those are given in Section 5.

Theorem 1.18 (Asymptotic formula for the radius). *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. Both $\liminf_{Z\to\infty} R^{\mathrm{HF}}_{Z,Z}(\nu)$ and $\limsup_{Z\to\infty} R^{\mathrm{HF}}_{Z,Z}(\nu)$ are bounded and behave asymptotically as*

$$3^{\frac{4}{3}} \frac{2^{\frac{1}{2}} \pi^{\frac{2}{3}}}{q^{\frac{2}{3}}} \nu^{-\frac{1}{3}} + o(\nu^{-\frac{1}{3}}) \text{ as } \nu \to \infty.$$

Theorem 1.19 (Bound on the ionization energy of a neutral atom). *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. The ionization energy of a neutral atom $E^{\mathrm{HF}}(Z-1, Z) - E^{\mathrm{HF}}(Z,Z)$ is bounded by a universal constant.*

Theorem 1.20 (Potential estimate). *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. For all $Z \geq 1$ and N with $N \geq Z$ for which a HF minimizer exists with $\int \rho^{\mathrm{HF}} = N$, we have*

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq A_\varphi |\mathbf{x}|^{-4+\varepsilon_0} + A_1,$$

with A_0, A_1 and ε_0 universal constants.

2 Prerequisites

In this section we recall some results that will be used in the rest of the paper. *Localization of the kinetic energy.* The following is the IMS formula corresponding to the operator $T(\mathbf{p})$.

Theorem 2.1 ([19]). *Let χ_i, $i = 0, \ldots, K$, be real valued Lipschitz continuous functions on $\mathbb{R}^3$ such that $\sum_{i=0}^K \chi_i^2(\mathbf{x}) = 1$ for all $\mathbf{x} \in \mathbb{R}^3$. Then for every $f \in H^{1/2}(\mathbb{R}^3)$*

$$\mathrm{t}(f,f) = \sum_{i=0}^{K} \mathrm{t}(\chi_i f, \chi_i f) - \alpha^{-1} \sum_{i=0}^{K} (f, L_i f),$$

where L_i is a bounded operator with kernel

$$L_i(\mathbf{x},\mathbf{y}) = \tfrac{\alpha^{-2}}{4\pi^2} \frac{|\chi_i(\mathbf{x}) - \chi_i(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|^2} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|), \tag{14}$$

where K_2 is a modified Bessel function of the second kind.

Remark 2.2. *As in [24, App.A, pages 94–98] we use the following integral formula for the modified Bessel function*

$$K_2(t) = t \int_0^\infty e^{-t\sqrt{s^2+1}} s^2 \, ds\,, \quad t > 0.$$

We recall that this function is decreasing and smooth in $\mathbb{R}^+$. Moreover,

$$\int_0^{+\infty} t^2 K_2(t)\, dt = \tfrac{3\pi}{2} \;\; \text{and} \;\; K_2(t) \le 16\, t^{-2} e^{-\frac{1}{2}t} \text{ for } t > 0. \tag{15}$$

The integral is computed in [21, (A6)] while the estimate follows directly from the integral formula for K_2 by estimating $\sqrt{s^2+1} \ge \frac{1}{2} + \frac{1}{2}s$.

Generalization of the Lieb-Thirring inequality. This result due to Daubechies generalizes the Lieb-Thirring inequality to the pseudo-relativistic case.

Theorem 2.3 (Daubechies' inequality, [4]). *For $\gamma \in \mathcal{A}$*

$$\mathrm{Tr}[T(\mathbf{p})\gamma] \ge \int_{\mathbb{R}^3} G_\alpha(\rho_\gamma(\mathbf{x})) d\mathbf{x},$$

where $G_\alpha(\rho) = \frac{3}{8}\alpha^{-4} C g(\alpha(\rho/C)^{\frac{1}{3}}) - \alpha^{-1}\rho$ with $C = .163q$, q the number of spin states and $g(t) = t(1+t^2)^{\frac{1}{2}}(1+2t^2) - \ln(t + (1+t^2)^{\frac{1}{2}})$.

Remark 2.4. *The function G_α defined in the previous theorem is convex and it has the following behavior:*

$$\tfrac{9}{20} \min\left\{ \tfrac{1}{5}\alpha C^{-\frac{2}{3}} \rho^{\frac{5}{3}}, \tfrac{1}{2} C^{-\frac{1}{3}} \rho^{\frac{4}{3}} \right\} \le G_\alpha(\rho) \le \tfrac{3}{2} \min\left\{ \tfrac{1}{5}\alpha C^{-\frac{2}{3}} \rho^{\frac{5}{3}}, \tfrac{1}{2} C^{-\frac{1}{3}} \rho^{\frac{4}{3}} \right\}. \tag{16}$$

(The proof of the estimate above is in Appendix A.) Notice that when $\alpha \searrow 0$ then $\alpha^{-1} G_\alpha(\rho)$ tends to a constant times $\rho^{5/3}$.

Theorem 2.5 (Generalization of the Lieb-Thirring inequality, [4]). *Let f^{-1} be the inverse of the function $f(t) := \sqrt{t^2+\alpha^{-2}} - \alpha^{-1}$, $t \geq 0$, and define $F(s) = \int_0^s dt\ [f^{-1}(t)]^3$. Then for any density matrix γ it holds*

$$\mathrm{Tr}[(T(\mathbf{p}) - U)\gamma] \geq -Cq \int_{\mathbb{R}^3} F(|U(\mathbf{x})|) d\mathbf{x},$$

with $C \leq 0.163$.

Remark 2.6. *Since $f^{-1}(t) = (t^2 + 2\alpha^{-1}t)^{1/2}$ we find for F*

$$F(s) = 2^{\frac{3}{2}} \alpha^{-3/2} \int_0^s t^{3/2} \big(1 + \tfrac{1}{2}\alpha t\big)^{3/2}\, dt \quad \text{for } s \geq 0, \tag{17}$$

and since by convexity $(1 + \frac{1}{2}\alpha t)^{\frac{3}{2}} \leq \sqrt{2} + \frac{1}{2}(\alpha t)^{\frac{3}{2}}$ we have

$$F(s) \leq \tfrac{2^3}{5} \alpha^{-\frac{3}{2}} s^{\frac{5}{2}} + \tfrac{1}{2\sqrt{2}} s^4 \text{ for } s \geq 0.$$

Hence for any density matrix γ and potential $U \in L^{\frac{5}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$

$$\mathrm{Tr}[(T(\mathbf{p}) - U)\gamma] \geq -Cq \int_{\mathbb{R}^3} \Big(\tfrac{2^3}{5} \alpha^{-\frac{3}{2}} |U(\mathbf{x})|^{\frac{5}{2}} + \tfrac{1}{2\sqrt{2}} |U(\mathbf{x})|^4) d\mathbf{x}. \tag{18}$$

Coulomb norm estimate. We present here only the definition of Coulomb norm and the result we need. For a more complete presentation we refer to [23, Sec.9].

Definition 2.7. *For $f, g \in L^{\frac{6}{5}}(\mathbb{R}^3)$ we define the Coulomb inner product*

$$D(f, g) := \tfrac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(\mathbf{x})\overline{g(\mathbf{y})}}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y},$$

and the corresponding norm $\|g\|_C := D(g, g)^{\frac{1}{2}}$.

In the following we write the direct term in the HF-energy functional using the Coulomb scalar product: i.e. $\mathcal{D}(\gamma) = D(\rho_\gamma, \rho_\gamma) = D(\rho_\gamma)$. Similarly, for $\rho \in L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3)$ the term $D(\rho)$ denotes $D(\rho, \rho)$.
The next proposition follows as Corollary 9.3 in [23].

Proposition 2.8. *For $s > 0$, $\mathbf{x} \in \mathbb{R}^3$ and $f \in L^{\frac{6}{5}}(\mathbb{R}^3)$ it holds*

$$f * |\mathbf{x}|^{-1} \leq \int_{|\mathbf{x}-\mathbf{y}|<s} [f(\mathbf{y})]_+ \Big(\frac{1}{|\mathbf{x} - \mathbf{y}|} - \frac{1}{s} \Big) d\mathbf{y} + \sqrt{2}\, s^{-\frac{1}{2}} \|f\|_C.$$

Moreover, for $k > 0$

$$\int_{|\mathbf{y}|<|\mathbf{x}|} \frac{f(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{y} \leq \int_{A(|\mathbf{x}|,k)} \frac{[f(\mathbf{y})]_+}{|\mathbf{x} - \mathbf{y}|} d\mathbf{y} + 2^{\frac{3}{2}} k^{-1} |\mathbf{x}|^{-\frac{1}{2}} \|f\|_C,$$

where $A(|\mathbf{x}|, k)$ denotes the annulus

$$A(|\mathbf{x}|, k) := \left\{ \mathbf{y} \in \mathbb{R}^3 : (1 - 2k)|\mathbf{x}| \leq |\mathbf{y}| \leq |\mathbf{x}| \right\}.$$

2.1 Improved relativistic Lieb-Thirring inequalities

A major difference between the pseudo-relativistic HF-model and the non-relativistic one studied in [23] is that the boundness of the functional does not yield a bound on the $L^{\frac{5}{3}}$ norm of the HF-density ρ^{HF} in the pseudo-relativistic case. By Theorem 2.3 and Remark 2.4 we see that we can control only the $L^{\frac{4}{3}}$-norm of ρ^{HF}. Therefore one cannot estimate the term $\rho^{\mathrm{HF}} * |\mathbf{x}|^{-1}$ in L^1-norm simply by Hölder's inequality with $p = 5/2$ and $q = 5/3$. To estimate it we are going to use a combined Daubechies-Lieb-Yau inequality.
The following lemma can be found in [24, pages 98–99][3].

Lemma 2.9. *For $f \in \mathcal{S}(\mathbb{R}^3)$,*

$$\int_{\mathbb{R}^3} \frac{e^{-\mu|\mathbf{x}|^2}}{|\mathbf{x}|}|f(\mathbf{x})|^2 d\mathbf{x} \leq \frac{\pi}{2}\frac{1}{\sqrt{2}-1}\,(f, T(\mathbf{p})f),$$

with $\mu = \pi^{-1}\alpha^{-2}$.

The following is a slight generalization of the Daubechies-Lieb-Yau inequality formulated in Theorem 2.8 in [24].

Theorem 2.10 (Daubechies-Lieb-Yau inequality). *Assume that the potential $U \in L^1_{loc}(\mathbb{R}^3)$ satisfies*

$$0 \geq -U(\mathbf{x}) \geq -\kappa|\mathbf{x}|^{-1} \quad \text{for } |\mathbf{x}| < \max\{\alpha, R\}\,, \tag{19}$$

for $\alpha, R > 0$ and $0 \leq \kappa \leq 2/\pi$. Then we have

$$\begin{aligned}\mathrm{Tr}[T(\mathbf{p}) - U]_- \quad &\geq \quad -C\kappa^{5/2}\alpha^{-3/2}R^{1/2} - C\kappa^4\alpha^{-1} \\ &\quad\; -C\int_{|\mathbf{x}|>R}\left(\alpha^{-\frac{3}{2}}|U(\mathbf{x})|^{\frac{5}{2}} + |U(\mathbf{x})|^4\right)d\mathbf{x}.\end{aligned}$$

Proof. If $(\sqrt{2}-1)/\pi \leq \kappa \leq 2/\pi$ then $\kappa^{5/2}\alpha^{-3/2}R^{1/2} + \kappa^4\alpha^{-1} \geq C\kappa^{5/2}\alpha^{-1}$ and the result follows immediately from Theorem 2.8 in [24] observing that for $R > \alpha$ the two integrals of the potential on $\{\alpha < |\mathbf{x}| < R\}$ are bounded by the constants.
If $0 \leq \kappa < (\sqrt{2}-1)/\pi$ we write

$$U(x) = e^{-\mu|x|^2}U(x)\chi_{|\mathbf{x}|<R} + (1 - e^{-\mu|x|^2})U(x)\chi_{|\mathbf{x}|<R} + U(x)\chi_{|\mathbf{x}|>R}$$

with $\mu = \alpha^{-2}\pi^{-1}$. Using (19) and Lemma 2.9 we find that

$$T(\mathbf{p}) - U(\mathbf{x}) \geq \frac{1}{2}T(\mathbf{p}) - \kappa(1 - e^{-\mu|\mathbf{x}|^2})|\mathbf{x}|^{-1}\chi_{|\mathbf{x}|<R} - U(\mathbf{x})\chi_{|\mathbf{x}|>R}.$$

[3] The result of the lemma and the proof given in [24] are actually due to us, but we communicated the result to the authors of [24], where it is referred to as a a private communication.

Hence from the generalization of the Lieb-Thirring inequality Theorem 2.5 (see (18)) we obtain

$$\begin{aligned}\mathrm{Tr}[T(\mathbf{p}) - U]_- \quad &\geq \quad -C\int_{|\mathbf{x}|<R} \alpha^{-\frac{3}{2}}\big(\kappa(1-e^{-\mu|\mathbf{x}|^2})|\mathbf{x}|^{-1})\big)^{\frac{5}{2}}\, d\mathbf{x} \\ & \quad -C\int_{|\mathbf{x}|<R} \big(\kappa(1-e^{-\mu|\mathbf{x}|^2})|\mathbf{x}|^{-1}\big)^{4}\, d\mathbf{x} \\ & \quad -C\int_{|\mathbf{x}|>R} \big(\alpha^{-\frac{3}{2}}|U(\mathbf{x})|^{\frac{5}{2}} + |U(\mathbf{x})|^4\big)\, d\mathbf{x}.\end{aligned}$$

Since the two first integrals above are estimated below by $-C\kappa^{5/2}\alpha^{-3/2}R^{1/2} - C\kappa^4\alpha^{-1}$ we get the result in the theorem. □

By Theorem 2.10 we find

$$\kappa\int_{|\mathbf{x}-\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \leq \mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] + C_1\kappa Z^{\frac{3}{2}}R^{\frac{1}{2}} + C_2\kappa^3 Z, \tag{20}$$

with $\kappa \in [0, 2/\pi]$, $\kappa = Z\alpha$ and $R > 0$ parameters to be chosen. This is the inequality that we use to estimate $\rho^{\mathrm{HF}} * |\mathbf{x}|^{-1}$ (see proof of Lemma 3.2 below).

2.1.1 Bound on the Hartree-Fock energy

As a first application of Theorem 2.10 we can give a lower bound to the HF-energy.

Theorem 2.11 (Bound on the HF-energy). *Let $N > 0$, $Z > 0$ and such that $Z\alpha = \kappa$ with $0 \leq \kappa \leq 2/\pi$. Then*

$$E^{\mathrm{HF}}(N, Z) \geq -2C^{\frac{2}{3}}Z^2N^{\frac{1}{3}} - C\kappa^2Z^2,$$

with C the constant in Theorem 2.10.

Proof. Let γ be a N-dimensional projection. Since the electron-electron interaction is positive we see that

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma) \quad &\geq \quad \alpha^{-1}\,\mathrm{Tr}[(T(\mathbf{p}) - \frac{Z\alpha}{|\cdot|})\gamma] \\ &= \quad \alpha^{-1}\,\mathrm{Tr}[(T(\mathbf{p}) - \frac{\kappa}{|\cdot|}\chi_{|\mathbf{x}|<R})\gamma] - \alpha^{-1}\,\mathrm{Tr}[\frac{\kappa}{|\cdot|}(1-\chi_{|\mathbf{x}|<R})\gamma]\end{aligned}$$

with $R > 0$ a parameter to be chosen. By Theorem 2.10 we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \quad \geq \quad -2C^{\frac{2}{3}}Z^2N^{\frac{1}{3}} - C\kappa^2Z^2,$$

using that $\kappa = Z\alpha$ and by choosing $R = C^{-\frac{2}{3}}Z^{-1}N^{\frac{2}{3}}$. □

3 Near the nucleus

In this section we prove the estimate in Theorem 1.17 in the region near the nucleus (i.e. at distance of $Z^{-\frac{1}{3}}$).
We again assume that $N \geq Z$ and that an HF-minimizer γ^{HF} exists for this N and Z. We denote the density of γ^{HF} by ρ^{HF}. We assume throughout that $\alpha Z = \kappa$ is fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$.

Lemma 3.1. *Let $Z\alpha = \kappa$ be fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. Let G_α be the function defined in Theorem 2.3. Then, there exists $\alpha_0 > 0$ such that for all $\alpha \leq \alpha_0$*

$$\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x} \leq CZ^{7/3}, \quad \alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] \leq CZ^{7/3}$$
$$\text{and} \quad \|\rho^{\mathrm{TF}} - \rho^{\mathrm{HF}}\|_C^2 \leq CZ^{2+\frac{3}{11}}, \tag{21}$$

with C a universal constant depending only on κ.

Proof. Let $\mu \in (0,1)$ be such that $\mu^{-1}\kappa < 2/\pi$. Notice that here we need $\kappa < 2/\pi$. Splitting the kinetic energy into two parts we find

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) &= (1-\mu)\alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] + \mathcal{D}(\gamma^{\mathrm{HF}}) - \mathcal{E}x(\gamma^{\mathrm{HF}}) \\ &\quad + \mu\operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - \frac{Z}{\mu|\mathbf{x}|})\gamma^{\mathrm{HF}}] = \dots,\end{aligned}$$

and introducing $\rho \in L^{\frac{5}{3}}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, $\rho \geq 0$, to be chosen

$$\begin{aligned}\dots &= (1-\mu)\alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] + \mu\|\rho - \rho^{\mathrm{HF}}\|_C^2 + (1-\mu)\mathcal{D}(\gamma^{\mathrm{HF}}) \\ &\quad - \mathcal{E}x(\gamma^{\mathrm{HF}}) - \mu D(\rho) + \mu\operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - (\frac{Z}{\mu|\mathbf{x}|} - \rho * \frac{1}{|\mathbf{x}|}))\gamma^{\mathrm{HF}}].\end{aligned} \tag{22}$$

Here $\|\cdot\|_C$ denotes the Coulomb norm defined in Definition 2.7 and we used that

$$\|\rho - \rho^{\mathrm{HF}}\|_C^2 = D(\rho) - \iint \frac{\rho^{\mathrm{HF}}(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y} + \mathcal{D}(\gamma^{\mathrm{HF}}).$$

The estimates in the claim will follow from (22) with different choices of μ and ρ. The main idea is to relate, up to lower order term, the last term on the right hand side of (22) to the TF-energy of a neutral atom of nuclear charge $Z\mu^{-1}$. This has been done in [21]. For completeness and easy reference we repeat the reasoning in Propositions B.1 and B.2 in Appendix B.
To prove the first inequality in (21) we choose ρ as the minimizer of the TF-energy functional of a neutral atom with charge $\mu^{-1}Z$. Since the corresponding TF-mean field potential is $Z/(\mu|\mathbf{x}|) - \rho * 1/|\mathbf{x}|$ by Proposition B.2 in Appendix B we find

$$\operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - (\frac{Z}{\mu|\mathbf{x}|} - \rho * \frac{1}{|\mathbf{x}|}))\gamma^{\mathrm{HF}}] \geq -C_1 Z^{\frac{7}{3}} + D(\rho). \tag{23}$$

Here we use (12). Since $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \leq 0$ from (22) and (23) leaving out the positive terms we find

$$0 \quad \geq \quad (1-\mu)\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] - \mathcal{E}x(\gamma^{\mathrm{HF}}) - C_1 Z^{\frac{7}{3}}. \tag{24}$$

From (24) and Theorem 2.3 we get

$$(1-\mu)\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} \leq (1-\mu)\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] \leq \mathcal{E}x(\gamma^{\mathrm{HF}}) + C_1 Z^{\frac{7}{3}}. \tag{25}$$

It remains to estimate the exchange term. By the exchange inequality (see [15])

$$\mathcal{E}x(\gamma^{\mathrm{HF}}) \quad \leq \quad 1.68\int_{\mathbb{R}^3}\big(\rho^{\mathrm{HF}}(\mathbf{x})\big)^{\frac{4}{3}}\,d\mathbf{x}.$$

To proceed we separate $\mathbb{R}^3$ into two regions. Let us define

$$\Sigma = \big\{\mathbf{x}\in\mathbb{R}^3 : \alpha\big(C^{-1}\rho^{\mathrm{HF}}(\mathbf{x})\big)^{\frac{1}{3}} \geq \tfrac{5}{2}\big\}, \tag{26}$$

with the same notation as in (16). By Remark 2.4, $G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x})) \geq C_2(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{4}{3}}$ in Σ and $\alpha^{-1}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x})) \geq C_3(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{5}{3}}$ in $\mathbb{R}^3\setminus\Sigma$. Hence by Hölder's inequality we find

$$\begin{aligned}\mathcal{E}x(\gamma^{\mathrm{HF}}) \quad &\leq \quad 1.68\int_{\Sigma}(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{4}{3}}\,d\mathbf{x}\\ &\qquad +1.68\Big(\int_{\mathbb{R}^3\setminus\Sigma}(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{5}{3}}\,d\mathbf{x}\Big)^{\frac{1}{2}}\Big(\int_{\mathbb{R}^3\setminus\Sigma}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}\Big)^{\frac{1}{2}}\\ &\leq C_4\int_{\mathbb{R}^3}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} + C_5\Big(\int_{\mathbb{R}^3}\alpha^{-1}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x}\Big)^{\frac{1}{2}}N^{\frac{1}{2}}.\end{aligned} \tag{27}$$

Choosing α_0 such that $1-\mu > 2C_4\alpha$ for $\alpha \leq \alpha_0$, from (25) and (27) we find

$$\tfrac{1-\mu}{2}\alpha^{-1}\int_{\mathbb{R}^3}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} \leq C_1 Z^{\frac{7}{3}} + C_5\Big(\int_{\mathbb{R}^3}\alpha^{-1}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x}\Big)^{\frac{1}{2}}N^{\frac{1}{2}}.$$

The first estimate in (21) follows from the estimate above using that $x^2-bx-c \leq 0$ implies $x^2 \leq b^2+2c$ and that $N \leq 2Z+1$ (Theorem 1.6). The second inequality in (21) follows then from (25) and the bound on the exchange term. To prove the third inequality in (21) we estimate from above and from below $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$. For the one from below we choose in (22) $\mu = 1$ and $\rho = \rho^{\mathrm{TF}}$ the TF-minimizer of a neutral atom with nucleus of charge Z. We find

$$\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = \sum_{i=1}^{N}(u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})u_i) + \|\rho^{\mathrm{HF}}-\rho^{\mathrm{TF}}\|_C^2 - D(\rho^{\mathrm{TF}}) - \mathcal{E}x(\gamma^{\mathrm{HF}}). \tag{28}$$

From (28) and the proof of Proposition B.2 (see (B37)), we find

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \quad \geq \quad & -\tfrac{2^{\frac{3}{2}}}{15\pi^2} q \int d\mathbf{q} (\varphi^{\mathrm{TF}}(\mathbf{q}))^{\frac{5}{2}} - C Z^{2+1/5} \\ & -D(\rho^{\mathrm{TF}}) + \|\rho^{\mathrm{HF}} - \rho^{\mathrm{TF}}\|_C^2 - \mathcal{E}x(\gamma^{\mathrm{HF}}).\end{aligned} \tag{29}$$

To estimate from above $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$ we may proceed exactly as in [23, page 543] using that $\alpha^{-1}T(\mathbf{p}) \leq \frac{1}{2}|\mathbf{p}|^2$. For completeness we repeat the main ideas. We consider γ the density matrix that acts identically on each of the spin components as

$$\gamma^j = \tfrac{1}{(2\pi)^3} \iint_{\frac{1}{2}|\mathbf{p}|^2 \leq \varphi^{\mathrm{TF}}(\mathbf{q})} \Pi_{\mathbf{p},\mathbf{q}} \, d\mathbf{q} d\mathbf{p} \text{ for } j = 1, \ldots, q.$$

Here $\Pi_{\mathbf{p},\mathbf{q}}$ is the projection onto the space spanned by $h_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) := h_s(\mathbf{x}-\mathbf{q})e^{i\mathbf{p}\cdot\mathbf{x}}$ where h_s is the ground state (normalized in $L^2(\mathbb{R}^3)$) for the Dirichlet Laplacian on the ball of radius Z^{-s} with $s \in (1/3, 2/3)$ to be chosen. One sees that $\mathrm{Tr}[\gamma] = Z \leq N$ since

$$\rho_\gamma(\mathbf{x}) = \tfrac{2^{3/2} q}{6\pi^2} (\varphi^{\mathrm{TF}})^{3/2} * h_s^2(\mathbf{x}) = \rho^{\mathrm{TF}} * h_s^2(\mathbf{x}),$$

where we have used the TF-equation. Hence $\mathcal{E}^{\mathrm{HF}}(\gamma) \geq \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$. Now we estimate from above $\mathcal{E}^{\mathrm{HF}}(\gamma)$. Since $\alpha^{-1}T(\mathbf{p}) \leq \frac{1}{2}|\mathbf{p}|^2$ and $\mathcal{E}x(\gamma) \geq 0$ we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \leq \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \frac{Z}{|\cdot|})\gamma] + D(\rho_\gamma) = \ldots,$$

and proceeding as in [23, page 543])

$$\cdots = \tfrac{q}{(2\pi)^3} \iint_{\frac{1}{2}|\mathbf{p}|^2 \leq \varphi^{\mathrm{TF}}(\mathbf{q})} \tfrac{1}{2}|\mathbf{p}|^2 \, d\mathbf{p} d\mathbf{q} - \tfrac{\pi^2}{2} Z^{2s} N - \int_{\mathbb{R}^3} \frac{Z}{|\mathbf{x}|} \rho_\gamma(\mathbf{x}) \, d\mathbf{x} + D(\rho_\gamma).$$

Computing the integral and summing and subtracting the term $\int \rho^{\mathrm{TF}} \varphi^{\mathrm{TF}}$ we get

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma) \quad \leq \quad & \tfrac{q 2^{\frac{1}{2}}}{5\pi^2} \int_{\mathbb{R}^3} (\varphi^{\mathrm{TF}}(\mathbf{q}))^{\frac{5}{2}} \, d\mathbf{q} - \tfrac{\pi^2}{2} Z^{2s} N - \int_{\mathbb{R}^3} \varphi^{\mathrm{TF}}(\mathbf{x}) \rho^{\mathrm{TF}}(\mathbf{x}) \, d\mathbf{x} \\ & - \int_{\mathbb{R}^3} \frac{Z}{|\mathbf{x}|} (\rho_\gamma(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})) d\mathbf{x} - 2D(\rho^{\mathrm{TF}}) + D(\rho_\gamma).\end{aligned} \tag{30}$$

By Newton's theorem one sees that $D(\rho_\gamma) \leq D(\rho^{\mathrm{TF}})$ and that

$$Z \int_{\mathbb{R}^3} \frac{\rho^{\mathrm{TF}}(\mathbf{x}) - \rho_\gamma(\mathbf{x})}{|\mathbf{x}|} \, d\mathbf{x} \leq Z \int_{|\mathbf{x}| \leq Z^{-s}} \frac{\rho^{\mathrm{TF}}(\mathbf{x})}{|\mathbf{x}|} \, d\mathbf{x} \leq C Z^{\frac{1}{5}(12-s)}.$$

In the last step we use Hölder's inequality and Corollary 1.15. From (30) using the TF-equation, that $N \leq 2Z + 1$ (Theorem 1.6) and optimizing in s we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \leq -\tfrac{2^{\frac{3}{2}}}{15\pi^2} q \int_{\mathbb{R}^3} (\varphi^{\mathrm{TF}}(\mathbf{q}))^{\frac{5}{2}} \, d\mathbf{q} + C Z^{\frac{1}{5}(12 - \frac{7}{11})} - D(\rho^{\mathrm{TF}}). \tag{31}$$

Hence from (29) and (31) we obtain

$$\left\|\rho^{\mathrm{HF}}-\rho^{\mathrm{TF}}\right\|_C^2 \leq C Z^{2+\frac{3}{11}}+\mathcal{E}x(\gamma^{\mathrm{HF}}).$$

The last estimate in (21) follows from the estimate above since $\mathcal{E}x(\gamma^{\mathrm{HF}}) \leq CZ^{\frac{5}{3}}$ using (27) and the estimate just proved on $\alpha^{-1}\int G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x}$. □

Lemma 3.2. *Let $Z\alpha=\kappa$ be fixed with $0\leq\kappa<2/\pi$ and $Z\geq 1$. Then, there exists an $\alpha_0>0$ such that for all $\alpha\leq\alpha_0$, $\mu>0$ and $\mathbf{x}\in\mathbb{R}^3$ with $|\mathbf{x}|\leq \beta Z^{-\frac{1+\mu}{3}}$ we have*

$$|\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})-\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{\frac{4}{1+\mu}}(1+\beta^{\frac{9}{22(1+\mu)}}|\mathbf{x}|^{\frac{2+11\mu}{22(1+\mu)}})|\mathbf{x}|^{-4+\frac{4\mu}{1+\mu}}.$$

Proof. By the definition of screened nuclear potential we have

$$\left|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})-\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})\right| \leq \int_{|\mathbf{y}|<|\mathbf{x}|}\frac{|\rho^{\mathrm{HF}}(\mathbf{y})-\rho^{\mathrm{TF}}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}=\dots$$

and for all $k>0$ by Proposition 2.8

$$\dots \leq 2^{\frac{3}{2}}k^{-1}|\mathbf{x}|^{-\frac{1}{2}}\left\|\rho^{\mathrm{HF}}-\rho^{\mathrm{TF}}\right\|_C+\int_{A(|\mathbf{x}|,k)}\frac{\rho^{\mathrm{HF}}(\mathbf{y})+\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}. \quad (32)$$

Since $\|\rho^{\mathrm{TF}}\|_{L^{\frac{5}{3}}(\mathbb{R}^3)}\leq CZ^{\frac{7}{5}}$ (Corollary 1.15) and

$$\int_{A(|\mathbf{x}|,k)}\frac{1}{|\mathbf{x}-\mathbf{y}|^{\frac{5}{2}}}d\mathbf{y}\leq 8\pi|\mathbf{x}|^{\frac{1}{2}}(2k)^{\frac{1}{2}}. \quad (33)$$

(see [23] page 549) one finds

$$\int_{A(|\mathbf{x}|,k)}\frac{\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \quad\leq\quad CZ^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}. \quad (34)$$

The term with the HF-density has to be treated differently since we do not have a bound for the $L^{\frac{5}{3}}$-norm of ρ^{HF}. For a $R\in\mathbb{R}^+$ to be chosen later we consider the splitting

$$\int_{A(|\mathbf{x}|,k)}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}=\int_{\substack{A(|\mathbf{x}|,k)\\|\mathbf{x}-\mathbf{y}|>R}}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}+\int_{\substack{A(|\mathbf{x}|,k)\\|\mathbf{x}-\mathbf{y}|<R}}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}. \quad (35)$$

We consider these two terms separately. Let Σ be defined as in (26); i.e. the region where $G_\alpha(\rho^{\mathrm{HF}})$ behaves like $(\rho^{\mathrm{HF}})^{\frac{4}{3}}$ (Remark 2.4). By Hölder's inequality we find

$$\begin{aligned}\int_{\substack{A(|\mathbf{x}|,k)\\|\mathbf{x}-\mathbf{y}|>R}}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \quad\leq\quad & \Big(\int_{\substack{A(|\mathbf{x}|,k)\\|\mathbf{x}-\mathbf{y}|>R}}\frac{1}{|\mathbf{x}-\mathbf{y}|^4}d\mathbf{y}\Big)^{\frac{1}{4}}\Big(\int_{\mathbf{y}\in\Sigma}(\rho^{\mathrm{HF}}(\mathbf{y}))^{\frac{4}{3}}d\mathbf{y}\Big)^{\frac{3}{4}}\\ &+\Big(\int_{A(|\mathbf{x}|,k)}\frac{1}{|\mathbf{x}-\mathbf{y}|^{\frac{5}{2}}}d\mathbf{y}\Big)^{\frac{2}{5}}\Big(\int_{\mathbf{y}\in\mathbb{R}^3\setminus\Sigma}(\rho^{\mathrm{HF}}(\mathbf{y}))^{\frac{5}{3}}d\mathbf{y}\Big)^{\frac{3}{5}}.\end{aligned}$$

From the inequality above, Remark 2.4 and estimate (21) we get

$$\int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \quad \leq \quad CR^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z + C|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}Z^{\frac{7}{5}}. \tag{36}$$

On the other hand for the second term on the right hand side of (35) by (20) and Lemma 3.1 we find

$$\int_{|\mathbf{x}-\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \leq C(Z^{\frac{4}{3}} + R^{\frac{1}{2}}Z^{\frac{3}{2}}). \tag{37}$$

Hence from (32), Lemma 3.1, (34), (36) and (37), we get

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\big(\frac{Z^{1+\frac{3}{22}}}{|\mathbf{x}|^{1/2}k} + Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}} + R^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z + R^{\frac{1}{2}}Z^{\frac{3}{2}} + Z^{\frac{4}{3}}\big). \tag{38}$$

Choosing k such that $Z^{\frac{4}{3}} = Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}$, i.e. $k = |\mathbf{x}|^{-1}Z^{-\frac{1}{3}}$ and R such that $R^{-\frac{3}{8}}Z^{1-\frac{1}{24}} = Z^{\frac{4}{3}}$, i.e. $R = Z^{-1}$ we find

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C(|\mathbf{x}|^{\frac{1}{2}}Z^{\frac{4}{3}+\frac{3}{22}} + Z^{\frac{4}{3}}).$$

The claim follows using that $|\mathbf{x}| \leq \beta Z^{-\frac{1+\mu}{3}}$. ☐

Theorem 3.3. *Let $Z\alpha = \kappa$ be fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. Then there exists an $\alpha_0 > 0$ such that for all $\alpha \leq \alpha_0$ and $\mathbf{x} \in \mathbb{R}^3$ with $|\mathbf{x}| \leq \beta Z^{-\frac{1}{3}}$ we have*

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{2-\frac{1}{66}}(1 + \beta^2 + \beta^{\frac{5}{2}} + \beta^{2+\frac{789}{1936}}|\mathbf{x}|^{\frac{179}{1936}})|\mathbf{x}|^{-4+\frac{1}{66}}. \tag{39}$$

Moreover if $|\mathbf{x}| \leq \beta Z^{-\frac{1-\mu}{3}}$ for $\mu < \frac{2}{11}\frac{1}{49}$, then

$$|\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{2-a(\mu)}(1 + \beta^2 + \beta^{\frac{5}{2}} + \beta^{b(\mu)}|\mathbf{x}|^{c(\mu)})|\mathbf{x}|^{-4+a(\mu)}, \tag{40}$$

with $a(\mu) = \frac{1}{66(1-\mu)} - \frac{49\mu}{12(1-\mu)}$, $b(\mu) = 2 + \frac{3}{176}\frac{24-24\mu-\frac{1}{11}+\frac{49}{2}\mu}{1-\mu}$ and $c(\mu) = \frac{1}{11} - \frac{\frac{3}{11}-\frac{3}{2}49\mu}{22(8-8\mu)}$ strictly positive constants.

Proof. Proceeding as in the proof of Lemma 3.2 up to (36) we get

$$\begin{aligned} |\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \quad &\leq \quad C(k^{-1}|\mathbf{x}|^{-\frac{1}{2}}Z^{1+\frac{3}{22}} + Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}} + R^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z) \\ &+ \quad \int_{|\mathbf{x}-\mathbf{y}|\leq R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}, \end{aligned} \tag{41}$$

for $R \in \mathbb{R}^+$ to be chosen. It remains to estimate the last term on the right hand side of (41). For 'small' R which is relevant for small $\mathbf{x}$ we already did it in Lemma 3.2, for 'big' R which is relevant for big $\mathbf{x}$ we use Proposition B.1 in Appendix B.

Take $\gamma \le 1/263$ to be chosen. If $|\mathbf{x}| \le \beta Z^{-\frac{1+\gamma}{3}}$ then by Lemma 3.2

$$|\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})| \le C\beta^{\frac{4}{1+\gamma}}(1+\beta^{\frac{9}{22(1+\gamma)}}|\mathbf{x}|^{\frac{2+11\gamma}{22(1+\gamma)}})|\mathbf{x}|^{-4+\frac{4\gamma}{1+\gamma}}. \tag{42}$$

If instead $|\mathbf{x}| > \beta Z^{-\frac{1+\gamma}{3}}$, let $H_{\mathbf{x}}$ be the Hamiltonian defined in (B2) with $\mathbf{P} = \mathbf{x}$ and $\nu = Z$. Then by the definition of $H_{\mathbf{x}}$ and taking the HF-minimizer as a trial wave function we have

$$\begin{aligned}\inf_{\substack{\psi\in\wedge_{i=1}^N L^2(\mathbb{R}^3)\\ \|\psi\|_2=1}} \langle\psi, H_{\mathbf{x}}\psi\rangle &\le \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) - Z\int_{|\mathbf{x}-\mathbf{y}|<R}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}\\ &= \inf_{\gamma\in\mathcal{A}}\mathcal{E}^{\mathrm{HF}}(\gamma) - Z\int_{|\mathbf{x}-\mathbf{y}|<R}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} = \dots .\end{aligned}$$

Since $\frac{1}{2}|\mathbf{p}|^2 \ge \alpha^{-1}T(\mathbf{p})$, $\inf_{\gamma\in\mathcal{A}}\mathcal{E}^{\mathrm{HF}}(\gamma)$ is estimated from above by the HF-ground state energy of the non-relativistic model (i.e. when the kinetic energy is given by $-\frac{1}{2}\Delta$). Moreover, this last one can be estimated from above by $\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) + CN^{\frac{1}{5}}Z^2$ (see [18] and [11]). Hence we find

$$\dots \le \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) + CN^{\frac{1}{5}}Z^2 - Z\int_{|\mathbf{x}-\mathbf{y}|<R}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}.$$

On the other hand since $|\mathbf{x}| > \beta Z^{-\frac{1+\gamma}{3}}$ choosing for some $l > \frac{1+\gamma}{3}$, $R < \beta Z^{-l}/4$ from Proposition B.1 it follows that there exists a constant depending only on κ such that for $t \in ((1+\gamma)/3, \min\{l, 3/5\})$, and for every $\psi \in \wedge_{i=1}^N L^2(\mathbb{R}^3)$ with $\|\psi\|_2 = 1$ we have

$$\langle\psi, H_{\mathbf{x}}\psi\rangle \ \ge\ \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - C(\beta^{1/2}+\beta^{-2})Z^{\frac{5}{2}-\frac{t}{2}},$$

Hence combining the two inequalities above we find

$$\int_{|\mathbf{x}-\mathbf{y}|\le R}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \le C(\beta^{1/2}+\beta^{-2})Z^{\frac{1}{2}(3-t)}. \tag{43}$$

From (41) and the inequality above we get

$$\begin{aligned}|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| &\le Ck^{-1}|\mathbf{x}|^{-\frac{1}{2}}Z^{1+\frac{3}{22}} + CZ^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}\\ &\quad + CR^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z + C(\beta^{1/2}+\beta^{-2})Z^{\frac{1}{2}(3-t)}.\end{aligned}$$

Choosing k such that $Z^{\frac{1}{2}(3-t)} = Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}$, i.e $k = |\mathbf{x}|^{-1}Z^{\frac{1}{2}(1-5t)}$ and R such that $Z^{\frac{1}{2}(3-t)} \sim R^{-\frac{3}{8}}Z^{1+\frac{1}{16}(1-5t)}$, i.e $R = \beta Z^{-\frac{7}{6}+\frac{1}{2}t}/4$ we find

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C(|\mathbf{x}|^{\frac{1}{2}}Z^{\frac{7}{11}+\frac{5}{2}t} + (\beta^{1/2}+\beta^{-2})Z^{\frac{1}{2}(3-t)}). \tag{44}$$

Notice that $R < \beta Z^{-l}/4$ is satisfied choosing $l = 4t/3$. Then for $\mathbf{x}$ such that $\beta Z^{-\frac{1+\gamma}{3}} \le |\mathbf{x}| \le \beta Z^{-\frac{1}{3}}$ we find

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C(|\mathbf{x}|^{-\frac{31}{22}-\frac{15}{2}t}\beta^{\frac{21}{11}+\frac{15}{2}t} + (\beta^{1/2}+\beta^{-2})\beta^{\frac{3}{2}(3-t)}|\mathbf{x}|^{-\frac{3}{2}(3-t)}).$$

Optimizing in t gives $t = 1/3 + 1/99$. For this value of t we get

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \le C(1+\beta^{\frac{5}{2}})\beta^{2-\frac{1}{66}}|\mathbf{x}|^{-4+\frac{1}{66}}. \qquad (45)$$

Inequality (39) follows from (42) and (45) choosing γ such that $4\gamma/(1+\gamma) = 1/66$, i.e. $\gamma = 1/263$.
On the other hand from (44) for $\mathbf{x}$ such that $\beta Z^{-\frac{1+\gamma}{3}} \le |\mathbf{x}| \le \beta Z^{-\frac{1-\mu}{3}}$ we find

$$\begin{aligned}|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \quad \le \quad & C|\mathbf{x}|^{\frac{1}{2}-\frac{3}{1-\mu}(\frac{7}{11}+\frac{5}{2}t)}\beta^{\frac{3}{1-\mu}(\frac{7}{11}+\frac{5}{2}t)} \\ & + C(\beta^{1/2}+\beta^{-2})\beta^{\frac{3}{2(1-\mu)}(3-t)}|\mathbf{x}|^{-\frac{3}{2(1-\mu)}(3-t)}.\end{aligned}$$

Optimizing in t gives $t = 1/3 + 1/99 - \frac{1}{18}\mu$. For this value of t we get

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \le C(1+\beta^{\frac{5}{2}})\beta^{2-\frac{1}{66(1-\mu)}+\frac{49\mu}{12(1-\mu)}}|\mathbf{x}|^{-4+\frac{1}{66(1-\mu)}-\frac{49\mu}{12(1-\mu)}}.$$

Inequality (40) follows from the one above and (42) choosing γ such that $4\gamma/(1+\gamma) = \frac{1}{66(1-\mu)} - \frac{49\mu}{12(1-\mu)}$. □

4 The exterior part

In this section we complete the proof of Theorem 1.17. We first estimate the exterior integral of the density and study the minimization problem that the exterior part of the minimizer satisfies. Then we prove the main estimate in Theorem 1.17 in an intermediate zone, i.e. far from the nucleus but not further than a fixed distance independent of Z. To study this area we need first to construct a TF-model that gives a good approximation of the HF-density in this intermediate zone. By the estimate on the exterior integral of the density we can then also prove Theorem 1.17 in the region far away from the nucleus.

4.1 The exterior integral of the density

The main result of this section is the following lemma.

Lemma 4.1 (The exterior integral of the density). *Assume that for some* $R, \sigma, \varepsilon' > 0$

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \le \sigma|\mathbf{x}|^{-4+\varepsilon'}, \qquad (46)$$

holds for $|\mathbf{x}| \le R$. *Then for* $0 < r \le R$

$$\Big|\int_{|\mathbf{x}|<r} (\rho^{\rm HF}(\mathbf{x}) - \rho^{\rm TF}(\mathbf{x}))\, d\mathbf{x}\Big| \le \sigma r^{-3+\varepsilon'} \qquad (47)$$

and

$$\int_{|\mathbf{x}|>r} \rho^{\rm HF}(\mathbf{x}) d\mathbf{x} \le C(1+\sigma r^{\varepsilon'})(1+r^{-3}), \qquad (48)$$

with C a universal constant.

We proceed similarly as in the proof of Lemma 10.5 in [23]. Since we need to localize we first present some technical lemmas that will take care of the error terms due to the localization. The localization error that will appear in the argument below (see (58)) will be in the form of an operator L similar to the error (14) in the IMS formula. We estimate this error in Lemma 4.3.

Remark 4.2. *Let $0 \leq \beta_1 < .. < \beta_4$ be real numbers with possibly $\beta_4 = \infty$. Let us denote $\Sigma_r(\beta_i, \beta_j) = \{\mathbf{x} \in \mathbb{R}^3 : \beta_i r \leq |\mathbf{x}| \leq \beta_j r\}$. Then we have*

$$\iint_{\substack{\mathbf{x} \in \Sigma_r(\beta_1,\beta_2) \\ \mathbf{y} \in \Sigma_r(\beta_3,\beta_4)}} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)^2 \, d\mathbf{x}d\mathbf{y} \leq \tfrac{4^6\pi^2}{3} \frac{\beta_2^3 - \beta_1^3}{\beta_3 - \beta_2} \, \alpha^4 r^2 e^{-\alpha^{-1} r(\beta_3 - \beta_2)} .$$

The proof of this estimate is given in Appendix A.

Lemma 4.3. *Let $r > 0$ and $\lambda, \nu \in (0,1)$. Let χ_- be the characteristic function of $B_{r(1-\nu)}(0)$ and χ_0 be the characteristic function of the sector $\{\mathbf{x} \in \mathbb{R}^3 : r(1-\nu) < |\mathbf{x}| < r(1+\nu)/(1-\lambda)\}$. Let η be a Lipschitz function such that $0 \leq \eta(\mathbf{x}) \leq 1$ for all $\mathbf{x} \in \mathbb{R}^3$, $\eta(\mathbf{x}) \equiv 0$ if $|\mathbf{x}| \leq r$, $\eta(\mathbf{x}) \equiv 1$ if $|\mathbf{x}| \geq r(1-\lambda)^{-1}$ and $\|\nabla \eta\|_\infty$ is bounded. Let L denote the operator with integral kernel*

$$L(\mathbf{x}, \mathbf{y}) = \frac{\alpha^{-2}}{4\pi^2} \frac{(\eta(\mathbf{x}) - \eta(\mathbf{y}))(\eta(\mathbf{x})|\mathbf{x}| - \eta(\mathbf{y})|\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|^2} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|). \tag{49}$$

Then for every function $f \in L^2(\mathbb{R}^3)$ we have

$$\alpha^{-1}|(f, Lf)| \leq 3\, D(\eta, \lambda, r)\, \|\chi_0 f\|_2^2 + D(\eta, \lambda, r) e^{-\frac{1}{2}\alpha^{-1} r\nu} \|\chi_- f\|_2^2 + \alpha^{-1}|(f, Qf)|,$$

with $D(\eta, \lambda, r) := \|\nabla \eta\|_\infty \Big(\frac{\|\nabla \eta\|_\infty r}{1-\lambda} + 1\Big)$ and Q a positive semi-definite operator such that

$$\mathrm{Tr}[Q] \leq C D(\eta, \lambda, r) \alpha^{-1} r^2 e^{-\frac{1}{2}\alpha^{-1} r\nu},$$

with C depending only on λ and ν.

Proof. As a first step we decompose the operator L. We introduce a third cut-off function χ_+ such that $1 = \chi_-(\mathbf{x}) + \chi_0(\mathbf{x}) + \chi_+(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^3$. We decompose the operator L with respect to these characteristic functions as follows:

$$L = \chi_- L(\chi_0 + \chi_+) + (\chi_0 + \chi_+) L \chi_- + \chi_0 L \chi_+ + \chi_+ L \chi_0 + \chi_0 L \chi_0.$$

We proceed similarly as in [24, Proof of Theorem 2.6 (Localization error)]. For Γ_1, Γ_2 bounded operators from $(\Gamma_1 - \Gamma_2)(\Gamma_1 - \Gamma_2)^* \geq 0$ it follows

$$\Gamma_1 \Gamma_2^* + \Gamma_2 \Gamma_1^* \leq \Gamma_1 \Gamma_1^* + \Gamma_2 \Gamma_2^*. \tag{50}$$

We are going to use several times this inequality with different choices of Γ_1 and Γ_2.

As a first choice we consider $\Gamma_1 = \sqrt{\varepsilon_1}\chi_-$ and $\Gamma_2 = 1/\sqrt{\varepsilon_1}(\chi_0+\chi_+)L\chi_-$ with $\varepsilon_1 > 0$ to be chosen. Using (50) we get

$$|(f, (\chi_- L(\chi_0+\chi_+) + (\chi_0+\chi_+)L\chi_-)f)| \leq \varepsilon_1 \|\chi_- f\|_2^2 + \frac{1}{\varepsilon_1}(f, Q_1 f), \tag{51}$$

with $Q_1 = (\chi_0+\chi_+)L\chi_-^2 L(\chi_0+\chi_+)$. We estimate now the trace of Q_1. By the definition of η, χ_-, χ_0 and χ_+ it follows that

$$\mathrm{Tr}[Q_1] = \int_{|\mathbf{x}|\leq r(1-\nu)} \int_{|\mathbf{y}|\geq r} L^2(\mathbf{x},\mathbf{y})\, d\mathbf{x}d\mathbf{y} \leq \tfrac{(16)^2}{3\pi^2} \tfrac{(1-\nu)^3}{\nu} D(\eta,\lambda,r)^2 r^2 e^{-\alpha^{-1}r\nu}.$$

In the last step we use the definition of L, Remark 4.2 and the definition of the constant $D(\eta,\lambda,r)$ given in the statement of the lemma.
Now we choose $\Gamma_1 = \sqrt{\varepsilon_2}\chi_0$ and $\Gamma_2 = 1/\sqrt{\varepsilon_2}\chi_+ L\chi_0$ with $\varepsilon_2 > 0$ to be chosen. Proceeding as above we get

$$|(f, (\chi_+ L\chi_0 + \chi_0 L\chi_+)f)| \leq \varepsilon_2 \|\chi_0 f\|_2^2 + \frac{1}{\varepsilon_2}(f, Q_2 f), \tag{52}$$

with $Q_2 = \chi_+ L\chi_0^2 L\chi_+$ and such that

$$\mathrm{Tr}[Q_2] \leq \tfrac{(16)^2}{3\pi^2} \tfrac{1-(1-\nu)^3(1-\lambda)^3}{\nu(1-\lambda)^2} D(\eta,\lambda,r)^2\ r^2 e^{-\alpha^{-1}r\frac{\nu}{1-\lambda}}.$$

It remains to study the term $\chi_0 L\chi_0$. This one has to be treated differently. By Schwartz's inequality one gets

$$|(f, \chi_0 L\chi_0 f)| \leq \tfrac{3\alpha}{2} D(\eta,\lambda,r) \int_{\mathbb{R}^3} \chi_0(\mathbf{x})|f(\mathbf{x})|^2, \tag{53}$$

since $\int_{\mathbb{R}^3} |L(\mathbf{x},\mathbf{y})| d\mathbf{x}d\mathbf{y} \leq \frac{3\alpha}{2} D(\eta,\lambda,r)$.
The claim follows from (51), (52) and (53) choosing $\varepsilon_1 = D(\eta,\lambda,r)\alpha e^{-\frac{1}{2}\alpha^{-1}r\nu}$, $\varepsilon_2 = \frac{3\alpha}{2} D(\eta,\lambda,r)$ and with $Q := \frac{1}{\varepsilon_1}Q_1 + \frac{1}{\varepsilon_2}Q_2$. □

Definition 4.4 (The localization function). *Fix $0 < \lambda < 1$ and let $G : \mathbb{R}^3 \to \mathbb{R}$ be given by*

$$G(\mathbf{x}) := \begin{cases} 0 & \text{if } |\mathbf{x}| \leq 1, \\ \frac{\pi}{2}(|\mathbf{x}|-1)\frac{1}{(1-\lambda)^{-1}-1} & \text{if } 1 \leq |\mathbf{x}| \leq (1-\lambda)^{-1}, \\ \frac{\pi}{2} & \text{if } (1-\lambda)^{-1} \leq |\mathbf{x}|. \end{cases}$$

Let $r > 0$ and define the outside localization function $\theta_r(\mathbf{x}) := \sin(G(\frac{|\mathbf{x}|}{r}))$.

Remark 4.5. *From the definition it follows that $\|\nabla\theta_r\|_\infty \leq \frac{\pi}{2}\frac{1-\lambda}{\lambda} r^{-1}$.*

Lemma 4.6. *For all $r > 0$ and $\lambda, \nu \in (0,1)$ the density ρ^{HF} of the minimizer satisfies*

$$\int_{|\mathbf{x}|>r(1-\lambda)^{-1}} \rho^{\mathrm{HF}}(\mathbf{x})d\mathbf{x} \quad\leq\quad 1 + \tfrac{2}{\lambda} + 2 \sup_{|\mathbf{x}|=r(1-\lambda)} |\mathbf{x}|\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x}) + \mathcal{R}^{\frac{1}{2}}$$

with

$$\mathcal{R} = 6D(\lambda)r^{-1}\int_{r(1-\nu)<|\mathbf{x}|<r\frac{1+\nu}{1-\lambda}} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} + 2D(\lambda)(r^{-1}N + Cr\alpha^{-2})e^{-\frac{1}{2}\alpha^{-1}r\nu},$$

with $D(\lambda) := (1+\pi/(2\lambda(1-\lambda)))\pi/(2\lambda)$ *and* $C = C(\lambda,\nu)$.

Proof. Let γ^{HF} be the minimizer. By the variational principle, γ^{HF} is a projection onto the subspace spanned by $u_1,\dots,u_N$. These functions u_i satisfy the Euler Lagrange equations $h_{\gamma^{\mathrm{HF}}}u_i = \varepsilon_i u_i$, $\varepsilon_i < 0$, for $i = 1,\dots,N$, with $h_{\gamma^{\mathrm{HF}}}$ defined in (11).
Given η a function in $C^1(\mathbb{R}^3)$ with support away from zero, we find

$$0 \geq \sum_{i=1}^{N}\varepsilon_i\int_{\mathbb{R}^3}|u_i(\mathbf{x})|^2|\mathbf{x}|\eta^2(\mathbf{x})d\mathbf{x} = \sum_{i=1}^{N}\int_{\mathbb{R}^3}u_i(\mathbf{x})^*|\mathbf{x}|\eta^2(\mathbf{x})\, h_{\gamma^{\mathrm{HF}}}u_i(\mathbf{x})d\mathbf{x}.$$

Since $\eta T(\mathbf{p})u_i \in L^2(\mathbb{R}^3)$ (Theorem 1.5, (3)), using the Euler-Lagrange equations and treating all the terms, except the kinetic energy, as in [23, Formula (63)] we get

$$\begin{aligned} 0 \;\geq\;& \alpha^{-1}\sum_{i=1}^{N}(u_i\eta|\cdot|, \eta T(\mathbf{p})u_i) - Z\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x} \\ &+\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\left[\rho^{\mathrm{HF}}(\mathbf{x})\rho^{\mathrm{HF}}(\mathbf{y}) - \mathrm{Tr}_{\mathbb{C}^q}|\gamma^{\mathrm{HF}}(\mathbf{x},\mathbf{y})|^2\right]\frac{|\mathbf{y}|(1-\eta^2(\mathbf{x}))\eta^2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y} \\ &+\tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2 - \tfrac{1}{2}\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}. \end{aligned} \tag{54}$$

Now we look at the kinetic energy term. For each $i \in \{1,\dots,N\}$ we may write

$$\mathrm{Re}(u_i\eta|\cdot|, \eta T(\mathbf{p})u_i) = \mathrm{Re}(u_i\eta|\cdot|, T(\mathbf{p})(\eta u_i)) + \mathrm{Re}(u_i\eta|\cdot|, [\eta, T(\mathbf{p})]u_i), \tag{55}$$

where $[A,B]$ denotes the commutator of the operators A and B. The first term on the right hand side of (55) is non-negative by the result of Lieb in [13]. Notice that here we may use that $\eta u_i \in H^1(\mathbb{R}^3)$ (see Theorem 1.5, (3)).
Hence, from (54) and (55) we find

$$\begin{aligned} 0 \;\geq\;& \alpha^{-1}\sum_{i=1}^{N}\mathrm{Re}(u_i\eta|\cdot|, [\eta, T(\mathbf{p})]u_i) - Z\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x} \\ &+\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\left[\rho^{\mathrm{HF}}(\mathbf{x})\rho^{\mathrm{HF}}(\mathbf{y}) - \mathrm{Tr}_{\mathbb{C}^q}|\gamma^{\mathrm{HF}}(\mathbf{x},\mathbf{y})|^2\right]\frac{|\mathbf{y}|(1-\eta^2(\mathbf{x}))\eta^2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y} \\ &+\tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2 - \tfrac{1}{2}\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}. \end{aligned} \tag{56}$$

By a density argument we may choose $\eta = \theta_r$ the localization function defined in Definition 4.4. Reasoning as on page 541 of [23], we get

$$\begin{aligned} 0 \quad \geq \quad & \alpha^{-1}\sum_{i=1}^{N} \mathrm{Re}(u_i\eta|\cdot|,[\eta,T(\mathbf{p})]u_i) + \tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2 \\ & -\Big(\tfrac{1}{2}+\tfrac{1}{\lambda}+\sup_{|\mathbf{x}|=r(1-\lambda)}|\mathbf{x}|\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})\Big)\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}. \end{aligned} \tag{57}$$

It remains to estimate the first term on the right hand side of (57). With the same arguments used in the proof of the IMS formula, it can be rewritten as

$$\alpha^{-1}\sum_{i=1}^{N}\mathrm{Re}(u_i\eta|\cdot|,[\eta,T(\mathbf{p})]u_i) = -\alpha^{-1}\sum_{i=1}^{N}(u_i,Lu_i), \tag{58}$$

where L is the operator defined in (49). Using Lemma 4.3 and since $\|\nabla\eta\|_\infty = \|\nabla\theta_r\|_\infty \leq \pi/(2\lambda r)$ we find, with $D(\lambda)$ defined as in the statement,

$$\begin{aligned} \alpha^{-1}\Big|\sum_{i=1}^{N}(u_i,Lu_i)\Big| \quad \leq \quad & 3D(\lambda)r^{-1}\|\chi_0\rho^{\mathrm{HF}}\|_1 + D(\lambda)r^{-1}e^{-\frac{1}{2}\alpha^{-1}r\nu}\|\chi_-\rho^{\mathrm{HF}}\|_1 \\ & + CD(\lambda)r\alpha^{-2}e^{-\frac{1}{2}\alpha^{-1}r\nu}, \end{aligned} \tag{59}$$

where χ_0, χ_- and C are as defined in the statement of Lemma 4.3. Hence combining (57) with (59), using the definition of χ_0 and that $\|\chi_-\rho^{\mathrm{HF}}\|_1 \leq N$ we have

$$\begin{aligned} 0 \quad \geq \quad & -3D(\lambda)r^{-1}\int_{r(1-\nu)<|\mathbf{x}|<r\frac{1+\nu}{1-\lambda}}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} - D(\lambda)r^{-1}e^{-\frac{1}{2}\alpha^{-1}r\nu}N \\ & -CD(\lambda)r\alpha^{-2}e^{-\frac{1}{2}\alpha^{-1}r\nu} + \tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2 \\ & -\Big(\tfrac{1}{2}+\tfrac{1}{\lambda}+\sup_{|\mathbf{x}|=r(1-\lambda)}|\mathbf{x}|\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})\Big)\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}. \end{aligned}$$

The claim follows using that $x^2 - Bx - C \leq 0$ implies $x \leq B + \sqrt{C}$. □

Proof of Lemma 4.1. We proceed as in [23, page 551]. The first estimate follows directly from the equality

$$\int_{|\mathbf{x}|<r}(\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))\,d\mathbf{x} = \tfrac{1}{4\pi}r\int_{S^2}(\Phi^{\mathrm{HF}}_r(r\omega) - \Phi^{\mathrm{TF}}_r(r\omega))\,d\omega,$$

and (46). To prove (48) we use Lemma 4.6. We first notice that for $0 < \beta < \gamma$

and γ such that $r\gamma \leq R$

$$\begin{aligned}\int_{r\beta<|\mathbf{y}|<r\gamma} \rho^{\mathrm{HF}}(\mathbf{y})\, d\mathbf{y} &\leq \Big|\int_{|\mathbf{y}|<r\gamma} (\rho^{\mathrm{HF}}(\mathbf{y}) - \rho^{\mathrm{TF}}(\mathbf{y}))\, d\mathbf{y}\Big| \\ &\quad + \Big|\int_{|\mathbf{y}|<r\beta} (\rho^{\mathrm{HF}}(\mathbf{y}) - \rho^{\mathrm{TF}}(\mathbf{y}))\, d\mathbf{y}\Big| + \int_{|\mathbf{y}|>r\beta} \rho^{\mathrm{TF}}(\mathbf{y})\, d\mathbf{y} \\ &\leq Cr^{-3}\beta^{-3}(1+\sigma r^{\varepsilon'}). \end{aligned} \tag{60}$$

Here we used (47) and that by the TF-equation and (13)

$$\int_{|\mathbf{y}|>r\beta} \rho^{\mathrm{TF}}(\mathbf{y})\, d\mathbf{y} \leq \tfrac{3^4 2\pi^2}{q^2}\beta^{-3}r^{-3}.$$

Since $\int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}} \leq \int_{|\mathbf{x}|>2r/3} \rho^{\mathrm{HF}}$ to prove the claim we estimate this second integral. By Lemma 4.6 with r replaced by $r/2$, $\lambda = \frac{1}{4}$ and $\nu = \frac{1}{2}$ we get

$$\int_{|\mathbf{x}|>2r/3} \rho^{\mathrm{HF}}(\mathbf{x})d\mathbf{x} \leq 9 + \tfrac{3}{4}r \sup_{|\mathbf{x}|=3r/8} \Phi^{\mathrm{HF}}_{3r/8}(\mathbf{x}) + \mathcal{R}^{\frac{1}{2}},$$

with $\mathcal{R}$ defined as in the statement of Lemma 4.6. By (46) and Corollary 1.14 we find

$$\sup_{|\mathbf{x}|=3r/8} \Phi^{\mathrm{HF}}_{3r/8}(\mathbf{x}) \leq C\sigma r^{-4+\varepsilon'} + \sup_{|\mathbf{x}|=3r/8} \Phi^{\mathrm{TF}}_{3r/8}(\mathbf{x}) \leq C(1+\sigma r^{\varepsilon'})r^{-4}.$$

Moreover, from (60) with $\beta = 1/4$ and $\gamma = 1$, since $N < 2Z+1$ and the boundness of $\mathbb{R}^+ \ni x \mapsto x^p e^{-x}$ for all $p > 0$, we find

$$\mathcal{R} \leq C(r^{-4}(1+\sigma r^{\varepsilon'}) + r^{-1}).$$

The claim follows directly. □

4.2 Separating the inside from the outside

We consider the exterior part of the minimizer, i.e. the density matrix

$$\gamma^{\mathrm{HF}}_r := \theta_r \gamma^{\mathrm{HF}} \theta_r, \tag{61}$$

with θ_r as defined in Definition 4.4. This density matrix almost minimizes a new energy functional where there is no exchange term. Indeed sufficiently far away from the nucleus the electrons are far apart and hence their mutual interaction is small.

We define an auxiliary energy functional on $\mathcal{A}$ (see (8)) given by

$$\mathcal{E}^A(\gamma) := \mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - \Phi^{\mathrm{HF}}_r)\gamma] + D(\rho_\gamma). \tag{62}$$

THEOREM 4.7. *Let $r > 0$ and $\lambda, \nu \in (0,1)$. Let χ_r^+ denote the characteristic function of $\mathbb{R}^3 \setminus B_r(0)$. The density matrix $\gamma_r^{\rm HF}$ defined in* (61) *satisfies*

$$\mathcal{E}^A(\gamma_r^{\rm HF}) \leq \Big\{ \mathcal{E}^A(\gamma) : \gamma \in \mathcal{A}, \mathrm{supp}(\rho_\gamma) \subset \mathbb{R}^3 \setminus B_r(0), \|\rho_\gamma\|_1 \leq \|\rho^{\rm HF}\chi_r\|_1 \Big\} + \mathcal{R},$$

where

$$\begin{aligned} \mathcal{R} \;\; = \;\; & (\tfrac{\pi}{2\lambda} + \tfrac{C}{\lambda^2} r^{-1}) r^{-1} \int_{r(1-\lambda)(1-\nu) \leq |\mathbf{x}|} \rho^{\rm HF}(\mathbf{x})\, d\mathbf{x} + c' \alpha^{-2}(1 + \alpha r^{-2}) e^{-\frac{1}{2}\alpha^{-1} r d} \\ & + \mathcal{E}x(\gamma_r^{\rm HF}) + C \int_{r(1-\lambda) \leq |\mathbf{x}| \leq \frac{r}{1-\lambda}} \Big[\big(\Phi^{\rm HF}_{r(1-\lambda)}(\mathbf{x})\big)^{\frac{5}{2}} + \alpha^3 \big(\Phi^{\rm HF}_{r(1-\lambda)}(\mathbf{x})\big)^4 \Big]\, d\mathbf{x}, \end{aligned}$$

and c', d are positive constants depending only on ν and λ.

Proof. We proceed as in [23, pages 532-6]. The first step of the proof is a localization. Once again we have to treat carefully the localization error coming from the kinetic energy. This is the main difference with [23]. For completeness we repeat the main ideas of the reasoning.

We consider the following partition of unity of $\mathbb{R}^3$: $1 = \theta_r^2(\mathbf{x}) + \theta_0^2(\mathbf{x}) + \theta_-^2(\mathbf{x})$ with θ_r defined as in Definition 4.4 and

$$\theta_0(\mathbf{x}) := \big(\theta^2_{r(1-\lambda)}(\mathbf{x}) - \theta_r^2(\mathbf{x})\big)^{\frac{1}{2}} \text{ and } \theta_-(\mathbf{x}) := \big(1 - \theta^2_{r(1-\lambda)}(\mathbf{x})\big)^{\frac{1}{2}}.$$

Associated to this partition of unity we define

$$\gamma_0^{\rm HF} := \theta_0 \gamma^{\rm HF} \theta_0 \text{ and } \gamma_-^{\rm HF} := \theta_- \gamma^{\rm HF} \theta_-.$$

We prove the claim by showing that for all density matrices $\gamma \in \mathcal{A}$ such that $\mathrm{supp}(\rho_\gamma) \subset \mathbb{R}^3 \setminus B_r(0)$ and $\|\rho_\gamma\|_1 \leq \|\rho^{\rm HF}\chi_r^+\|_1$ it holds that

$$\mathcal{E}^A(\gamma_r^{\rm HF}) + \mathcal{E}^{\rm HF}(\gamma_-^{\rm HF}) - \mathcal{R} \leq \mathcal{E}^{\rm HF}(\gamma^{\rm HF}) \leq \mathcal{E}^A(\gamma) + \mathcal{E}^{\rm HF}(\gamma_-^{\rm HF}). \tag{63}$$

The proof of the upper bound in (63) is as in [23, page 533].

To prove the lower bound as a first step we localize. By Theorem 2.1 we find

$$\begin{aligned} \alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\rm HF}] \;\; = \;\; & \alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})(\gamma_r^{\rm HF} + \gamma_0^{\rm HF} + \gamma_-^{\rm HF})] \\ & - \alpha^{-1} \sum_{i=1}^N (u_i, (L_r + L_0 + L_-) u_i), \end{aligned}$$

where L_r, L_0 and L_- are defined as the L_i's in (14).

We first estimate the error term. The procedure is similar to the one used in the proof of Lemma 4.3. We introduce three cut-off functions: χ_- be the characteristic function of $B_{r(1-\lambda)(1-\nu)}(0)$, χ_r the characteristic function of $\mathbb{R}^3 \setminus B_{r\frac{1+\nu}{1-\lambda}}(0)$ and χ_0 defined by $\chi_0(\mathbf{x}) = 1 - \chi_r(\mathbf{x}) - \chi_-(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^3$. Notice that χ_- and χ_r are the characteristic functions of sets where θ_-, θ_0 and θ_r are constants. For $k \in \{-, 0, r\}$ we have the following splitting

$$L_k = \chi_- L_k(\chi_0 + \chi_r) + (\chi_0 + \chi_r) L_k \chi_- + \chi_r L_k \chi_0 + \chi_0 L_k \chi_r + \chi_0 L_k \chi_0,$$

and proceeding as in the proof of Lemma 4.3 with $\varepsilon_{1,k}, \varepsilon_{2,k}$ to be chosen we find

$$\begin{aligned}(f, L_k f) \quad &\leq \quad \varepsilon_{1,k}\|\chi_- f\|_2^2 + \varepsilon_{1,k}^{-1}(f, Q_1 f) + \varepsilon_{2,k}\|\chi_0 f\|_2^2 + \varepsilon_{2,k}^{-1}(f, Q_2 f) \\ &\quad + \tfrac{3\alpha}{2}\|\nabla\theta_k\|_\infty^2 \|\chi_0 f\|_2^2.\end{aligned}$$

with operators Q_1 and Q_2 being positive semi-definite operators with

$$\begin{aligned}\mathrm{Tr}[Q_1] \quad &\leq \quad \tfrac{(16)^2}{3\pi^2}\tfrac{(1-\lambda)^2(1-\nu)^3}{\nu}\|\nabla\theta_k\|_\infty^4 r^2 e^{-\alpha^{-1} r\nu(1-\lambda)} \\ \mathrm{Tr}[Q_2] \quad &\leq \quad \tfrac{(16)^2}{3\pi^2}\tfrac{1}{\nu(1-\lambda)^2}\|\nabla\theta_k\|_\infty^4 r^2 e^{-\alpha^{-1} r \frac{\nu}{1-\lambda}}.\end{aligned}$$

Choosing then

$$\varepsilon_{2,k} = \tfrac{3\alpha}{2}\|\nabla\theta_k\|_\infty^2 \text{ and } \varepsilon_{1,k} = \alpha\|\nabla\theta_k\|_\infty^2 e^{-\frac{1}{2}\alpha^{-1} r\nu(1-\lambda)},$$

since $(\|\nabla\theta_r\|_\infty^2 + \|\nabla\theta_0\|_\infty^2 + \|\nabla\theta_-\|_\infty^2) \leq 3\pi^2/(4\lambda^2)r^{-2}$ and $\|\rho^{\mathrm{HF}}\chi_-\|_1 \leq N$ we get

$$\begin{aligned}\alpha^{-1}\sum_{i=1}^{N}(u_i, (L_r + L_0 + L_-)u_i) \quad &\leq \quad \tfrac{3\pi^2}{4\lambda^2} r^{-2}\|\rho^{\mathrm{HF}}\chi_0\|_1 + \tfrac{3\pi^2}{4\lambda^2} r^{-2} e^{-\frac{1}{2}\alpha^{-1} r\nu(1-\lambda)} N \\ &\quad + \quad c\alpha^{-2} e^{-\frac{1}{2}\alpha^{-1} r\nu(1-\lambda)}.\end{aligned}$$

Here c is a constant that depends only on ν and λ.
Hence from (64), the inequality above and since $N \leq 2Z + 1$ we find

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \quad &\geq \quad \mathrm{Tr}\left[\left(\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\cdot|}\right)(\gamma_r^{\mathrm{HF}} + \gamma_0^{\mathrm{HF}} + \gamma_-^{\mathrm{HF}})\right] + \mathcal{D}(\gamma^{\mathrm{HF}}) \\ &\quad -\mathcal{E}x(\gamma^{\mathrm{HF}}) - \tfrac{3\pi^2}{4\lambda^2} r^{-2}\|\rho^{\mathrm{HF}}\chi_0\|_1 - c'\alpha^{-2}(1 + \alpha r^{-2}) e^{-\frac{1}{2}\alpha^{-1} r d}.\end{aligned}$$

The constants c', d depend only on λ and ν. Proceeding as in [23] we get

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \quad &\geq \quad \mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) + \mathcal{E}^{A}(\gamma_r^{\mathrm{HF}}) - \mathcal{E}x(\gamma_r^{\mathrm{HF}}) - c'\alpha^{-2}(1 + \alpha r^{-2}) e^{-\frac{1}{2}\alpha^{-1} r d} \\ &\quad + \mathrm{Tr}\left[\left(\alpha^{-1}T(\mathbf{p}) - \Phi_{r(1-\lambda)}^{\mathrm{HF}}(\cdot)\right)\gamma_0^{\mathrm{HF}}\right] \\ &\quad -(\tfrac{\pi}{2\lambda} + \tfrac{3\pi^2}{4\lambda^2} r^{-1}) r^{-1}\int_{|\mathbf{x}|\geq r(1-\lambda)(1-\nu)} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x}.\end{aligned}$$

The claim follows using Theorem 2.5. □

4.3 Comparing with an Outside Thomas Fermi

At this point we introduce an "Outside Thomas Fermi": a TF-energy functional whose minimizer approximates the HF-density at a certain distance from the nucleus.

Let $r > 0$ such that

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le \sigma |\mathbf{x}|^{-4+\varepsilon'}, \tag{64}$$

for all $|\mathbf{x}| \le r$ for some $\sigma > 0$ and $\varepsilon' > 0$. Let V_r be the potential defined by

$$V_r(\mathbf{x}) = \chi_r^+(\mathbf{x})\Phi_r^{\mathrm{HF}}(\mathbf{x}) = \begin{cases} 0 & \text{if } |\mathbf{x}| < r, \\ \Phi_r^{\mathrm{HF}}(\mathbf{x}) & \text{if } |\mathbf{x}| \ge r. \end{cases} \tag{65}$$

Here and in the following $\chi_r^+(\mathbf{x}) := 1 - \chi_r(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$, where χ_r is the characteristic function of the ball of radius r centered at 0. Notice that $V_r \in L^{\frac{5}{2}}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with

$$\inf\{\|W\|_\infty : V_r - W \in L^{\frac{5}{2}}(\mathbb{R}^3)\} = 0.$$

Let $\mathcal{E}_r^{\mathrm{OTF}}$ be the TF-functional $\mathcal{E}_{V_r}^{\mathrm{TF}}$ corresponding to the potential V_r defined in (65). Let ρ_r^{OTF} be the unique minimizer of $\mathcal{E}_r^{\mathrm{OTF}}$ under the condition

$$\int_{\mathbb{R}^3} \rho(\mathbf{x}) d\mathbf{x} \le \int_{|\mathbf{y}|\ge r} \rho^{\mathrm{HF}}(\mathbf{y}) d\mathbf{y},$$

(see Theorem 1.9). Then ρ_r^{OTF} is solution to the OTF-equation

$$\tfrac{1}{2}\left(\tfrac{6\pi^2}{q}\right)^{\frac{2}{3}} (\rho_r^{\mathrm{OTF}})^{\frac{2}{3}} = [\varphi_r^{\mathrm{OTF}} - \mu_r^{\mathrm{OTF}}]_+ , \tag{66}$$

where

$$\varphi_r^{\mathrm{OTF}}(\mathbf{x}) = V_r(\mathbf{x}) - \int_{\mathbb{R}^3} \frac{\rho_r^{\mathrm{OTF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y},$$

is the OTF-mean field potential and μ_r^{OTF} is the corresponding chemical potential. From (66) (and $\mu_r^{\mathrm{OTF}} \ge 0$) we see that the support of ρ_r^{OTF} is contained in $\mathbb{R}^3 \setminus B_r(0)$.

In the intermediary zone instead of comparing directly $\Phi^{\mathrm{HF}}_{|\mathbf{x}|}$ and $\Phi^{\mathrm{TF}}_{|\mathbf{x}|}$ we compare first the HF-density with the OTF-density and then the OTF-density with the TF-density. When comparing the TF and OTF there is no difference with the non-relativistic case and for brevity we refer for the proofs to [23].

We start by studying the behavior of the minimizer and mean field potential of the OTF. The proof of the following bounds is in [23, page 557-558] in the case $q = 2$ and it can be directly generalised to the other values of q.

Lemma 4.8 ([23, Lem.12.1]). *For all $\mathbf{y} \in \mathbb{R}^3$ we have*

$$\varphi^{\mathrm{TF}}(\mathbf{y}) \le 3^4 2^{-1} q^{-2} \pi^2 |\mathbf{y}|^{-4} \text{ and } \rho^{\mathrm{TF}}(\mathbf{y}) \le 3^5 2^{-1} q^{-2} \pi |\mathbf{y}|^{-6}.$$

Let β_0 be as defined in Theorem 1.12, then for all $|\mathbf{y}| \ge \beta_0 Z^{-\frac{1}{3}}$ we have

$$\varphi^{\mathrm{TF}}(\mathbf{y}) \ge C|\mathbf{y}|^{-4} \text{ and } \rho^{\mathrm{TF}}(\mathbf{y}) \ge C|\mathbf{y}|^{-6}.$$

With r, σ, ε' such that (64) holds and $\sigma r^{\varepsilon'} \le 1$ we have for all $|\mathbf{y}| \ge r$

$$\rho_r^{\mathrm{OTF}}(\mathbf{y}) \le Cr^{-6} \text{ and } \varphi_r^{\mathrm{OTF}}(\mathbf{y}) \le |V_r(\mathbf{y})| \le Cr^{-4}.$$

Lemma 4.9 ([23, Lem.12.2]). *With r, σ, ε' such that* (64) *holds for all* $|\mathbf{x}| \le r$ *we have*

$$\int_{|\mathbf{y}|\ge r} (\rho^{\mathrm{TF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y} \le \sigma r^{-3+\varepsilon'}.$$

For $\mathbf{x} \in \mathbb{R}^3$ with $|\mathbf{x}| > r$ we may write

$$\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) = \mathcal{A}_1(r,\mathbf{x}) + \mathcal{A}_2(r,\mathbf{x}) + \mathcal{A}_3(r,\mathbf{x}), \tag{67}$$

where

$$\begin{aligned} \mathcal{A}_1(r,\mathbf{x}) &= \varphi^{\mathrm{OTF}}_r(\mathbf{x}) - \varphi^{\mathrm{TF}}(\mathbf{x}), \\ \mathcal{A}_2(r,\mathbf{x}) &= \int_{|\mathbf{y}|>|\mathbf{x}|} \frac{\rho^{\mathrm{OTF}}_r(\mathbf{y}) - \rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \end{aligned}$$

and

$$\mathcal{A}_3(r,\mathbf{x}) = \int_{r<|\mathbf{y}|<|\mathbf{x}|} \frac{\rho^{\mathrm{OTF}}_r(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}.$$

4.3.1 Estimate on $\mathcal{A}_1$ and $\mathcal{A}_2$

Lemma 4.10 ([23, Lem.12.4]). *Let $N \ge Z$. Given $\varepsilon', \sigma > 0$ there exists a constant $D > 0$ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which* (64) *holds for all $|\mathbf{x}| \le r$, then $\mu^{\mathrm{OTF}}_r = 0$ and*

$$\tfrac{3^4\pi^2}{2q^2}|\mathbf{x}|^{-4}(1 + ar^{\zeta}|\mathbf{x}|^{-\zeta})^{-2} \le \varphi^{\mathrm{OTF}}_r(\mathbf{x}) \le \tfrac{3^4\pi^2}{2q^2}|\mathbf{x}|^{-4}(1 + Ar^{\zeta}|\mathbf{x}|^{-\zeta}) \quad \textit{for } |\mathbf{x}| > r,$$

where a, A are universal constants and $\zeta = (-7+\sqrt{73})/2$.

Lemma 4.11 ([23, Lem.12.5]). *Let $N \ge Z$. Given $\varepsilon', \sigma > 0$ there exists a constant $D > 0$ depending only on ε', σ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which* (64) *holds for $|\mathbf{x}| \le r$, then for all $|\mathbf{x}| \ge r$*

$$|\mathcal{A}_1(r,\mathbf{x})| \le C|\mathbf{x}|^{-4-\zeta}r^{\zeta} \quad \textit{and} \quad |\mathcal{A}_2(r,\mathbf{x})| \le C|\mathbf{x}|^{-4-\zeta}r^{\zeta},$$

with $\zeta = (-7+\sqrt{73})/2$ and C a universal constant.

The proof of the previous lemmas is in [23, p. 558-564].

4.3.2 Estimate on $\|\chi^+_r\rho^{\mathrm{HF}} - \rho^{\mathrm{OTF}}_r\|_C$

Lemma 4.12. *Let G_α be the function defined in Theorem 2.3 and $\rho^{\mathrm{HF}}_r(\mathbf{x})$ be the one-particle density of the density matrix γ^{HF}_r defined in* (61). *Let $Z\alpha = \kappa$ fixed, $0 \le \kappa < 2/\pi$ and $Z \ge 1$.*
Given constants $\varepsilon', \sigma > 0$ there exists $D < \frac{4}{5}$ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which (64) *holds for $|\mathbf{x}| \le r$, it follows that*

$$\begin{aligned} \alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}_r(\mathbf{x}))\, d\mathbf{x} &\le \alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}_r] \\ &\le 2\mathcal{R} + Cr^{-7} + Cr^{-4}\int_{\mathbb{R}^3} \rho^{\mathrm{HF}}_r(\mathbf{x})\, d\mathbf{x}, \end{aligned}$$

with C a universal positive constant and $\mathcal{R}$ as defined in Theorem 4.7.

Proof. The first inequality follows directly from Theorem 2.3. To prove the second inequality we proceed as in Lemma 3.1. In this case we are interested only in the exterior part of the minimizer. Hence, instead of considering the HF-energy functional we consider the auxiliary functional $\mathcal{E}^A$, defined in (62), applied to the "exterior part of the minimizer" $\gamma_r^{\rm HF}$.
Splitting the kinetic energy in two terms we find

$$\mathcal{E}^A(\gamma_r^{\rm HF}) \geq \tfrac{1}{2}\alpha^{-1}\,{\rm Tr}[T(\mathbf{p})\gamma_r^{\rm HF}] + D(\rho_r^{\rm HF}) + \tfrac{1}{2}\,{\rm Tr}[(\alpha^{-1}T(\mathbf{p}) - 2\Phi_r^{\rm HF})\gamma_r^{\rm HF}]. \quad (68)$$

Since $\Phi_r^{\rm HF}(\mathbf{x})$ is harmonic for $|\mathbf{x}| > r$ and going to zero at infinity

$$\Phi_r^{\rm HF}(\mathbf{x}) \leq \frac{r}{|\mathbf{x}|}\sup_{|\mathbf{y}|=r}\Phi_r^{\rm HF}(\mathbf{y}) \ \text{ for } |\mathbf{x}| > r.$$

Hence, since ${\rm supp}(\rho_r^{\rm HF}) \subset \mathbb{R}^3 \setminus B_r(0)$ we find

$${\rm Tr}[(\alpha^{-1}T(\mathbf{p}) - 2\Phi_r^{\rm HF})\gamma_r^{\rm HF}] \geq {\rm Tr}[(\alpha^{-1}T(\mathbf{p}) - \frac{2r}{|\cdot|}\sup_{|\mathbf{y}|=r}\Phi_r^{\rm HF}(\mathbf{y}))\gamma_r^{\rm HF}] = \ldots.$$

Adding and subtracting $2D(\rho, \rho_r^{\rm HF})$ for $\rho \in L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3)$, $\rho \geq 0$, to be chosen

$$\ldots \;=\; {\rm Tr}[(\alpha^{-1}T(\mathbf{p}) - V_\rho)\gamma_r^{\rm HF}] - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_r^{\rm HF}(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}. \quad (69)$$

where for simplicity of notation here and in the following V_ρ is defined as $V_\rho(\mathbf{x}) := \frac{2r}{|\mathbf{x}|}\sup_{|\mathbf{y}|=r}\Phi_r^{\rm HF}(\mathbf{y}) - \rho * \frac{1}{|\mathbf{x}|}$.
From (69), (68) and the definition of the Coulomb norm and scalar product (Definition 2.7) we find

$$\begin{aligned}\mathcal{E}^A(\gamma_r^{\rm HF}) \;&\geq\; \tfrac{1}{2}\alpha^{-1}\,{\rm Tr}[T(\mathbf{p})\gamma_r^{\rm HF}] + \tfrac{1}{2}D(\rho_r^{\rm HF}) + \tfrac{1}{2}\|\rho_r^{\rm HF} - \rho\|_C^2 \\ &\quad -\tfrac{1}{2}D(\rho) + \tfrac{1}{2}\,{\rm Tr}[(\alpha^{-1}T(\mathbf{p}) - V_\rho)\gamma_r^{\rm HF}] \qquad (70) \\ &\geq\; \tfrac{1}{2}\alpha^{-1}\,{\rm Tr}[T(\mathbf{p})\gamma_r^{\rm HF}] + \tfrac{1}{2}\sum_{i=1}^N(\theta_r u_i, (\alpha^{-1}T(\mathbf{p}) - V_\rho)\theta_r u_i) - \tfrac{1}{2}D(\rho),\end{aligned}$$

denoting by u_i the HF-orbitals.
We now choose ρ as the minimizer of the TF-energy functional of a neutral atom with Coulomb potential and nuclear charge $2r\sup_{|\mathbf{y}|=r}\Phi_r^{\rm HF}(\mathbf{y})$. Then V_ρ is the corresponding TF-mean field potential and we see that the last two terms on the right hand side of (70) are like the ones in the claim of Proposition B.2. The only difference is due to the presence of the localization function θ_r. We now prove that these terms give the TF-energy modulo lower order terms. The method is the same as that of Proposition B.2. We repeat the main steps since in this case the scaling depends on r. Notice that since $r > \beta_0 Z^{-\frac{1}{3}}$ the contribution is coming only from the "outer zone".

Let $g \in C_0^\infty(\mathbb{R}^3)$ be spherically symmetric, normalized in $L^2(\mathbb{R}^3)$ and with support in $B_1(0)$. Let us define $g_r(\mathbf{x}) := r^{-3}g(\mathbf{x}r^{-2})$ and $\psi_r := g_r^2$. Since V_ρ is sub-harmonic on $|\mathbf{x}| > 0$, we see from the support properties of ψ_r and θ_r that

$$\sum_{i=1}^N (\theta_r u_i, (\alpha^{-1}T(\mathbf{p}) - V_\rho)\theta_r u_i) \geq \sum_{i=1}^N (\theta_r u_i, (\alpha^{-1}T(\mathbf{p}) - V_\rho * \psi_r)\theta_r u_i) = \dots .$$

For $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ we define the coherent states $g_r^{\mathbf{p},\mathbf{q}}(\mathbf{x}) := g_r(\mathbf{x} - \mathbf{q})e^{i\mathbf{p}\cdot\mathbf{x}}$. By the formulas (B16) and (B17) with $L_\mathbf{q}$ the operator defined in the equation below (B17) we get

$$\begin{aligned} \dots \quad = \quad & \tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{p}d\mathbf{q}\, (T(\mathbf{p}) - \alpha V_\rho(\mathbf{q})) \sum_{i=1}^N \sum_{j=1}^q |(\theta_r u_i^j, g_r^{\mathbf{p},\mathbf{q}})|^2 \\ & - \alpha^{-1}\sum_{i=1}^N \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{x}d\mathbf{q}\, \overline{(\theta_r u_i)}(\mathbf{x})(L_\mathbf{q}\theta_r u_i)(\mathbf{x})\,, \end{aligned} \tag{71}$$

where u_i^j denotes the j-th spin component of the orbital u_i. By the choice of the function g_r and with the same arguments that led to (B19) in the appendix we find

$$\begin{aligned} & \alpha^{-1}\sum_{i=1}^N \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{x}d\mathbf{q}\, \overline{(\theta_r u_i)}(\mathbf{x})(L_\mathbf{q}\theta_r u_i)(\mathbf{x}) \\ \leq \quad & 3\sum_{i=1}^N \|\theta_r u_i\|_2^2 \|\nabla g_r\|_\infty^2 Vol(\mathrm{supp}(g_r)) \leq Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1. \end{aligned} \tag{72}$$

In the first term on the right hand side of (71) the integrand is zero if $|\mathbf{q}| < \frac{1}{4}r^2$ since in this case $\mathrm{supp}(\theta_r) \cap \mathrm{supp}(g_r^{\mathbf{q},\mathbf{p}}) = \emptyset$ (by the choice $D < 4/5$). To estimate it further from below we consider only the negative part of the integrand

$$\begin{aligned} & \tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{p}d\mathbf{q}\, (T(\mathbf{p}) - \alpha V_\rho(\mathbf{q})) \sum_{i=1}^N \sum_{j=1}^q |(\theta_r u_i^j, g_r^{\mathbf{p},\mathbf{q}})|^2 \\ \geq \quad & \tfrac{q}{(2\pi)^3}\alpha^{-1} \iint_{\substack{|\mathbf{q}| > \frac{1}{4}r^2 \\ T(\mathbf{p}) \leq \alpha V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\, (T(\mathbf{p}) - \alpha V_\rho(\mathbf{q}))\,, \end{aligned} \tag{73}$$

where we have used that $0 \leq \sum_{i=1}^N |(\theta_r u_i^j, g_r^{\mathbf{p},\mathbf{q}})|^2 \leq 1$ (Bessel's inequality). We split the domain of integration in $\mathbf{p}$ as follows

$$\{\mathbf{p} \in \mathbb{R}^3 : T(\mathbf{p}) \leq \alpha V_\rho(\mathbf{q})\} = \Sigma_1 \cup \Sigma_2$$

with Σ_1, Σ_2 disjoint and $\Sigma_1 = \{\mathbf{p} \in \mathbb{R}^3 : \frac{1}{2}|\mathbf{p}|^2 \leq V_\rho(\mathbf{q})\}$. We treat these two contributions separately. We have

$$\alpha^{-1}\iint_{\substack{|\mathbf{q}| > \frac{1}{4}r^2 \\ \mathbf{p} \in \Sigma_2}} d\mathbf{p}d\mathbf{q}\, (T(\mathbf{p}) - \alpha V_\rho(\mathbf{q})) \geq -\iint_{\substack{|\mathbf{q}| > \frac{1}{4}r^2 \\ \mathbf{p} \in \Sigma_2}} d\mathbf{p}d\mathbf{q}\, [V_\rho(\mathbf{q})]_+ = \dots$$

and computing the integral, using that $(1+x)^{\frac{3}{2}} \le 1 + \frac{3}{2}x + \frac{3}{8}x^2$

$$\cdots \ge -C \int_{|\mathbf{q}|>\frac{1}{4}r^2} d\mathbf{q}\, (\alpha^2 [V_\rho(\mathbf{q})]_+^{\frac{7}{2}} + \alpha^4 [V_\rho(\mathbf{q})]_+^{\frac{9}{2}}) \ge -C\alpha^2 r^{-\frac{23}{2}} - C\alpha^4 r^{-\frac{33}{2}}. \tag{74}$$

In the last step we used that $[V_\rho(\mathbf{q})]_+ \le 2\frac{r}{|\mathbf{q}|} \sup_{|\mathbf{x}|=r} \Phi_r^{\mathrm{HF}}(\mathbf{x})$ and that by the hypothesis and Corollary 1.14

$$r \sup_{|\mathbf{x}|=r} \Phi_r^{\mathrm{HF}}(\mathbf{x}) \le Cr^{-3}, \tag{75}$$

choosing D such that $\sigma r^{\varepsilon'} \le 1$.
Since $T(\mathbf{p}) \ge \frac{1}{2}\alpha|\mathbf{p}|^2 - \frac{1}{8}\alpha^3|\mathbf{p}|^4$ we find

$$\begin{aligned} &\alpha^{-1} \iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \mathbf{p}\in\Sigma_1}} d\mathbf{p}d\mathbf{q}\, (T(\mathbf{p}) - \alpha V_\rho(\mathbf{q})) \\ \ge\ & \iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \frac{1}{2}|\mathbf{p}|^2 \le V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\, (\frac{1}{2}|\mathbf{p}|^2 - V_\rho(\mathbf{q})) - \tfrac{1}{8}\alpha^2 \iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \frac{1}{2}|\mathbf{p}|^2 \le V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\, |\mathbf{p}|^4. \end{aligned} \tag{76}$$

Computing the last integral we find

$$\alpha^2 \iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \frac{1}{2}|\mathbf{p}|^2 \le V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\, |\mathbf{p}|^4 \le C\alpha^2 r^{-1} (2r \sup_{|\mathbf{x}|=r} \Phi_r^{\mathrm{HF}}(\mathbf{x}))^{\frac{7}{2}} \le C\alpha^2 r^{-\frac{23}{2}}. \tag{77}$$

While for the first term on the right hand side of (76), computing the integral with respect to $\mathbf{p}$, we get

$$\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \frac{1}{2}|\mathbf{p}|^2 \le V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\, (\tfrac{1}{2}|\mathbf{p}|^2 - V_\rho(\mathbf{q})) = -4\pi \frac{2^{\frac{5}{2}}}{15} \int_{|\mathbf{q}|>\frac{1}{4}r^2} d\mathbf{q}\, [V_\rho(\mathbf{q})]_+^{\frac{5}{2}}.$$

Hence collecting together (71), (72), (73) (74), (77) and the inequality above we find

$$\mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - V_\rho)\gamma_r^{\mathrm{HF}}] \ge -\frac{2^{\frac{3}{2}}q}{15\pi^2} \int_{\mathbb{R}^3} d\mathbf{x}\, [V_\rho(\mathbf{x})]_+^{\frac{5}{2}} - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1 - Cr^{-\frac{11}{2}} = \ldots.$$

since $\beta_0 Z^{-\frac{1}{3}} \le r$ implies $\beta_0\alpha^{\frac{1}{3}} \le \kappa^{\frac{1}{3}} r$. From the TF-equation that ρ satisfies it follows that

$$\begin{aligned} \ldots &= \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}} \int_{\mathbb{R}^3} d\mathbf{x}\, \rho(\mathbf{x})^{\frac{5}{3}} - \int_{\mathbb{R}^3} \rho(\mathbf{x}) V_\rho(\mathbf{x})\, d\mathbf{x} - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1 - Cr^{-\frac{11}{2}} \\ &= \mathcal{E}^{\mathrm{TF}}(\rho) + D(\rho) - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1 - Cr^{-\frac{11}{2}}. \end{aligned}$$

Hence from (70) and the inequality above we get using (12) and (75)

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \ \ge\ \tfrac{1}{2}\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] - Cr^{-7} - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1.$$

The claim follows since $\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \le \mathcal{R}$ by the result of Theorem 4.7 considering as a trial density matrix $\gamma \equiv 0$. □

Lemma 4.13. *Let $N' \in \mathbb{N}$ and $Z\alpha = \kappa$ be fixed, $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. Let e_j be the first N' negative eigenvalues of the operator $\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}$ acting on functions with support on $\{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \geq r\}$.*
Given constants $\varepsilon', \sigma > 0$ there exists $D < 4/5$ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \leq r \leq D$ for which (64) holds for $|\mathbf{x}| \leq r$, for all $\mu \in (0,1)$ and $s < r$ we have

$$\begin{aligned}\sum_{j=1}^{N'} e_j \quad &\geq \quad -(\tfrac{2}{1-\mu})^{\frac{3}{2}} \tfrac{1}{15\pi^2} \int_{|\mathbf{q}|>r} [\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\, d\mathbf{q} - Cr^{-8} s\mu^{-\frac{3}{2}} - C\mu^{-3} r^{-5} s \\ &\quad -C(1-\mu)^{-\frac{7}{2}} r^{-5} - C(1-\mu)s^{-2}N',\end{aligned}$$

with C a positive constant.

Proof. Let f_j be the eigenfunctions (normalized in $L^2(\mathbb{R}^3, \mathbb{C}^q)$) corresponding to the eigenvalues e_j, $j = 1, .., N'$. Let $g \in C_0^\infty(\mathbb{R}^3)$ with support in $B_1(0)$ and define $g_s(\mathbf{x}) = s^{-\frac{3}{2}} g(\mathbf{x}/s)$ for a positive parameter s, $s < r$. We then write for $\mu \in (0,1)$

$$\sum_{j=1}^{N'} e_j = \sum_{j=1}^{N'} (f_j, (\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}) f_j) = \mathcal{B}_1 + \mathcal{B}_2,$$

where

$$\begin{aligned}\mathcal{B}_1 \quad &= \quad \sum_{j=1}^{N'} (f_j, ((1-\mu)\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}} * g_s^2) f_j), \\ \mathcal{B}_2 \quad &= \quad \sum_{j=1}^{N'} (f_j, (\mu\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}} + \varphi_r^{\mathrm{OTF}} * g_s^2) f_j).\end{aligned}$$

We estimate these two terms separately. Considering for $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ the coherent states $g_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) := e^{i\mathbf{p}\cdot\mathbf{x}} g_s(\mathbf{x} - \mathbf{q})$ using (B16) and (B17), we find

$$\begin{aligned}\mathcal{B}_1 \quad &= \quad \tfrac{1}{(2\pi)^3} \iint ((1-\mu)\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q})) \sum_{j=1}^{N} |(f_j, g_s^{\mathbf{p},\mathbf{q}})|^2\, d\mathbf{q} d\mathbf{p} \\ &\quad - (1-\mu)\alpha^{-1} \sum_{j=1}^{N'} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} d\mathbf{x} d\mathbf{q} \overline{f_j(\mathbf{x})} (L_{\mathbf{q}} f_j)(\mathbf{x})\,. \qquad (78)\end{aligned}$$

Estimating the error term as done in (B32) and previous inequalities we get

$$(1-\mu)\alpha^{-1} \sum_{j=1}^{N'} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} d\mathbf{x} d\mathbf{q} \overline{f_j(\mathbf{x})} (L_{\mathbf{q}} f_j)(\mathbf{x}) \leq C(1-\mu)s^{-2}N'.$$

Since we are interested in an estimate from below and $\varphi_r^{\mathrm{OTF}}(\mathbf{q}) \leq 0$ for $|\mathbf{q}| < r$, from (78) we find

$$\mathcal{B}_1 \geq \frac{1}{(2\pi)^3}\iint_{|\mathbf{q}|>r}((1-\mu)\alpha^{-1}T(\mathbf{p})-\varphi_r^{\mathrm{OTF}}(\mathbf{q}))\sum_{j=1}^{N}|(f_j,g_s^{\mathbf{p},\mathbf{q}})|^2\,d\mathbf{q}d\mathbf{p} -C(1-\mu)s^{-2}N'. \tag{79}$$

We estimate now the first term on the right hand side of (79). Considering only the negative part of the integrand and since $\sum_{j=1}^{N'}|(f_j,g_s^{\mathbf{p},\mathbf{q}})|^2\leq 1$ we get

$$\begin{aligned} &\frac{1}{(2\pi)^3}\iint_{|\mathbf{q}|>r}((1-\mu)\alpha^{-1}T(\mathbf{p})-\varphi_r^{\mathrm{OTF}}(\mathbf{q}))\sum_{j=1}^{N'}|(f_j,g_s^{\mathbf{p},\mathbf{q}})|\,d\mathbf{q}d\mathbf{p} \\ \geq\ &\frac{1}{(2\pi)^3}\iint_{\substack{|\mathbf{q}|>r,\\ (1-\mu)\alpha^{-1}T(\mathbf{p})\leq\varphi_r^{\mathrm{OTF}}(\mathbf{q})}}((1-\mu)\alpha^{-1}T(\mathbf{p})-\varphi_r^{\mathrm{OTF}}(\mathbf{q}))\,d\mathbf{p}d\mathbf{q}. \end{aligned}$$

Now we split the domain of integration in $\mathbf{p}$ as follows

$$\{\mathbf{p}\in\mathbb{R}^3:\alpha^{-1}(1-\mu)T(\mathbf{p})\leq\varphi_r^{\mathrm{OTF}}(\mathbf{q})\}=\Sigma_1\cup\Sigma_2,$$

with Σ_1,Σ_2 disjoint and $\Sigma_1=\{\mathbf{p}\in\mathbb{R}^3:(1-\mu)|\mathbf{p}|^2/2\leq\varphi_r^{\mathrm{OTF}}(\mathbf{q})\}$. We treat these two contributions separately. Then

$$\begin{aligned} &\frac{1}{(2\pi)^3}\iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_2}}((1-\mu)\alpha^{-1}T(\mathbf{p})-\varphi_r^{\mathrm{OTF}}(\mathbf{q}))d\mathbf{p}d\mathbf{q} \\ \geq\ &-\frac{1}{(2\pi)^3}\iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_2}}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+d\mathbf{p}d\mathbf{q}=\dots \end{aligned}$$

and since in the domain of integration

$$\tfrac{2}{1-\mu}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+\leq|\mathbf{p}|^2\leq\tfrac{2}{1-\mu}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+(1+\tfrac{1}{2(1-\mu)}\alpha^2[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+)$$

we get

$$\begin{aligned} \dots\ \geq\ &-\frac{C}{(1-\mu)^{\frac52}}\alpha^2\int_{|\mathbf{q}|>r}d\mathbf{q}\,([\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac72}+\tfrac{\alpha^2}{8(1-\mu)}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac92}) \\ \geq\ &-\frac{C}{(1-\mu)^{\frac52}}\alpha^2(r^{-11}+\tfrac{\alpha^2}{1-\mu}r^{-15}), \end{aligned} \tag{80}$$

using Lemma 4.10 in the last step.
Since $\sqrt{1+t^2}\geq 1+(1/2)t^2-(1/8)t^4$, we get

$$\begin{aligned} &\frac{1}{(2\pi)^3}\iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_1}}((1-\mu)\alpha^{-1}T(\mathbf{p})-\varphi_r^{\mathrm{OTF}}(\mathbf{q}))d\mathbf{p}d\mathbf{q} \\ \geq\ &\frac{1}{(2\pi)^3}\iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_1}}((1-\mu)\tfrac12|\mathbf{p}|^2-\varphi_r^{\mathrm{OTF}}(\mathbf{q})-\tfrac18(1-\mu)\alpha^2|\mathbf{p}|^4)d\mathbf{p}d\mathbf{q}. \end{aligned}$$

The last term gives by Lemma 4.10

$$\alpha^2 \iint_{\substack{|\mathbf{q}|>r\\ \mathbf{p}\in\Sigma_1}} d\mathbf{p}d\mathbf{q}\, |\mathbf{p}|^4 = \alpha^2 \tfrac{4\pi}{7} \int_{|\mathbf{q}|>r} d\mathbf{q}\, (\tfrac{2}{1-\mu})^{\frac{7}{2}} [\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{7}{2}} \leq C\alpha^2 (\tfrac{2}{1-\mu})^{\frac{7}{2}} r^{-11}. \tag{81}$$

While for the other terms computing the integral with respect to $\mathbf{p}$, we get

$$\begin{aligned} &\tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_1}} ((1-\mu)\tfrac{1}{2}|\mathbf{p}|^2 - \varphi_r^{\mathrm{OTF}}(\mathbf{q}))d\mathbf{p}d\mathbf{q} \\ &= -(\tfrac{2}{1-\mu})^{\frac{3}{2}} \tfrac{1}{15\pi^2} \int_{|\mathbf{q}|>r} d\mathbf{q}\, [\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}. \end{aligned} \tag{82}$$

For the term $\mathcal{B}_2$ using Theorem 2.5 and Remark 2.6 we find

$$\mathcal{B}_2 \geq -Cq(\mu^{-\frac{3}{2}} \|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_{\frac{5}{2}}^{\frac{5}{2}} + \alpha^3\mu^{-3} \|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_4^4).$$

From the choice of g_s it follows that $\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2 \leq V_r - V_r * g_s^2$ and the term $V_r - V_r * g_s^2$ is non-zero only for $r - s \leq |\mathbf{x}| \leq r + s$. Hence by Lemma 4.8 and since $s < r$

$$\|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_{\frac{5}{2}}^{\frac{5}{2}} \leq \int_{r-s\leq|\mathbf{x}|\leq r+s} [V_r(\mathbf{x}) - V_r * g^2(\mathbf{x})]_+^{\frac{5}{2}} d\mathbf{x} \leq Cr^{-8}s, \tag{83}$$

and similarly $\|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_4^4 \leq Cr^{-14}s$. The claim follows from (79), (80), (81), (82) and (83) using that $\beta_0\alpha^{\frac{1}{3}} \leq \kappa^{\frac{1}{3}} r$. □

Lemma 4.14. *Let G_α be the function defined in Theorem 2.3 and $\rho_r^{\mathrm{HF}}(\mathbf{x})$ the one-particle density of the density matrix γ_r^{HF} defined in* (61)*. Let $Z\alpha = \kappa$ be fixed, $0 \leq \kappa < 2/\pi$ and $Z \geq 1$.*
There exists $\alpha_0 > 0$ such that given $\varepsilon', \sigma > 0$ there exists $D < 1/4$ such that for all $\alpha \leq \alpha_0$ and r with $\beta_0 Z^{-\frac{1}{3}} \leq r \leq D$ for which (64) *holds for $|\mathbf{x}| \leq r$, we have*

$$\begin{aligned} &\|\chi_r^+\rho^{\mathrm{HF}} - \rho_r^{\mathrm{OTF}}\|_C \leq Cr^{-\frac{7}{2}+\frac{1}{6}} \qquad \textit{and} \\ &\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\chi_r^+\rho^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x} \leq Cr^{-7}, \quad \alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma_r^{\mathrm{HF}}] \leq Cr^{-7}, \end{aligned} \tag{84}$$

with C a universal positive constant.

Proof. The idea of the proof is the same as that of Lemma 3.1. In this case we are interested only in the exterior part of the minimizer. Hence, instead of considering the HF-energy functional we estimate from above and below the auxiliary one $\mathcal{E}^A$, defined in (62), applied on the "exterior part of the minimizer" γ_r^{HF}.
Step I. Estimate from above on $\mathcal{E}^A(\gamma_r^{\mathrm{HF}})$. Let us consider γ the density matrix that acts identically on the spin components and on each as

$$\gamma^j = \tfrac{1}{(2\pi)^3} \iint_{\frac{1}{2}|\mathbf{p}|^2 \leq \varphi_r^{\mathrm{OTF}}(\mathbf{q})} \Pi_{\mathbf{p},\mathbf{q}}\, d\mathbf{p}d\mathbf{q},$$

where $j \in \{1, \ldots, q\}$ is the spin index, $\Pi_{\mathbf{p},\mathbf{q}}$ is the projection onto the space spanned by $h_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) = h_s(\mathbf{x}-\mathbf{q})e^{i\mathbf{p}\cdot\mathbf{x}}$ where h_s is the ground state for the Dirichlet Laplacian on the ball of radius s for $0 < s < r$. By the OTF-equation (66) and since $\mu_r^{\mathrm{OTF}} = 0$ (see Lemma 4.10) we see that $\rho_\gamma(\mathbf{x}) = \rho_r^{\mathrm{OTF}} * |h_s|^2(\mathbf{x})$. Moreover, by Lemma 4.10

$$\mathrm{Tr}[-\tfrac{1}{2}\Delta\gamma] = \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}} \int_{\mathbb{R}^3} (\rho_r^{\mathrm{OTF}}(\mathbf{x}))^{\frac{5}{3}}\, d\mathbf{x} + Cs^{-2}r^{-3}. \tag{85}$$

Since $[\Phi_r^{\mathrm{HF}}]_+ \in L^{\frac{5}{2}}_{loc}(\mathbb{R}^3)$, by [23, Lemma 8.5] for $\lambda' \in (0,1)$ we may find $\tilde\gamma$ such that $\mathrm{supp}(\rho_{\tilde\gamma}) \subset \{\mathbf{x} : |\mathbf{x}| \geq r\}$, $\rho_{\tilde\gamma}(\mathbf{x}) \leq \rho_\gamma(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^3$ and

$$\begin{aligned}\mathrm{Tr}[(-\tfrac{1}{2}\Delta - \Phi_r^{\mathrm{HF}})\tilde\gamma] \quad &\leq \quad \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \chi_r^+\Phi_r^{\mathrm{HF}})\gamma] + L_1 \int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} [V_r(\mathbf{x})]_+^{\frac{5}{2}}\, d\mathbf{x} \\ &\quad + \tfrac{1}{2}(\tfrac{\pi}{2\lambda' r})^2 \int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} \rho_\gamma(\mathbf{x})\, d\mathbf{x}. \end{aligned} \tag{86}$$

Since $\int \rho_{\tilde\gamma} \leq \int \rho_\gamma = \int \rho_r^{\mathrm{OTF}} \leq \int \chi_r^+ \rho^{\mathrm{HF}}$ we may choose $\tilde\gamma$ as a trial density matrix in Theorem 4.7 and we find for λ, ν to be chosen

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \leq \mathcal{E}^A(\tilde\gamma) + \mathcal{R} \leq \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \Phi_r^{\mathrm{HF}})\tilde\gamma] + \mathcal{R} + D(\rho_{\tilde\gamma}),$$

since $\alpha^{-1}T(\mathbf{p}) \leq \frac{1}{2}|\mathbf{p}|^2$. Notice that $\mathcal{R}$ depends on λ and ν. From (86) it follows that

$$\begin{aligned}\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \quad &\leq \quad \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \chi_r^+\Phi_r^{\mathrm{HF}})\gamma] + L_1 \int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} [V_r(\mathbf{x})]_+^{\frac{5}{2}}\, d\mathbf{x} \\ &\quad + \tfrac{1}{2}(\tfrac{\pi}{2\lambda' r})^2 \int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} \rho_\gamma(\mathbf{x})\, d\mathbf{x} + \mathcal{R} + D(\rho_{\tilde\gamma}). \end{aligned} \tag{87}$$

From the OTF-equation (66) and Lemma 4.10 we get

$$\int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} \rho_\gamma(\mathbf{x})\, d\mathbf{x} \leq \int_{|\mathbf{x}|\leq \frac{2-\lambda'}{1-\lambda'}r} \rho_r^{\mathrm{OTF}}(\mathbf{x})\, d\mathbf{x} \leq Cr^{-3}.$$

While since $V_r(\mathbf{y}) \leq Cr^{-4}$ (Lemma 4.8) and is non-zero only for $|\mathbf{y}| > r$

$$\int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} [V_r(\mathbf{x})]_+^{\frac{5}{2}}\, d\mathbf{x} \leq Cr^{-7}\tfrac{\lambda'}{(1-\lambda')^3}.$$

Hence, from (85) and (87) and the inequalities above we find choosing $\lambda' = r^{\frac{2}{3}}$

$$\begin{aligned}\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \quad &\leq \quad \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}} \int_{\mathbb{R}^3} (\rho_r^{\mathrm{OTF}}(\mathbf{x}))^{\frac{5}{3}}\, d\mathbf{x} - \int_{\mathbb{R}^3} V_r(\mathbf{x})\rho_\gamma(\mathbf{x})\, d\mathbf{x} + Cs^{-2}r^{-3} \\ &\quad + Cr^{-7+\frac{2}{3}} + \mathcal{R} + D(\rho_{\tilde\gamma}) = \ldots. \end{aligned}$$

Here we used that $\lambda' \leq 1/2$ which follows by the bound on D. Since $\rho_{\tilde\gamma} \leq \rho_\gamma$, $D(\rho_{\tilde\gamma}) \leq D(\rho_\gamma)$. Moreover by Newton's Theorem $D(\rho_\gamma) \leq D(\rho_r^{\rm OTF})$. Hence we get

$$\begin{aligned} \ldots \quad \leq \quad & \mathcal{E}^{\rm OTF}(\rho_r^{\rm OTF}) + \int_{\mathbb{R}^3} V_r(\mathbf{x})(\rho_r^{\rm OTF}(\mathbf{x}) - \rho_\gamma(\mathbf{x}))\, d\mathbf{x} + Cs^{-2}r^{-3} \\ & + Cr^{-7+\frac{2}{3}} + \mathcal{R}. \end{aligned} \tag{88}$$

We study now the second term on the right hand side of (88). Since $\rho_\gamma = \rho^{\rm OTF} * |h_s|^2$, rewriting

$$\int_{\mathbb{R}^3} V_r(\mathbf{x})(\rho_r^{\rm OTF}(\mathbf{x}) - \rho_\gamma(\mathbf{x}))\, d\mathbf{x} = \int_{\mathbb{R}^3} \rho_r^{\rm OTF}(\mathbf{x})(V_r(\mathbf{x}) - V_r * |h_s|^2(\mathbf{x}))\, d\mathbf{x}.$$

Since $s < r$, V_r is harmonic on $|\mathbf{x}| > r$ and $\rho_r^{\rm OTF}$ vanishes for $|\mathbf{x}| < r$ one sees that the integrand on the right hand side of the equation above is non-zero only for $r < |\mathbf{x}| < r + s$. Hence by Lemma 4.8

$$\int_{\mathbb{R}^3} V_r(\mathbf{x})(\rho_r^{\rm OTF}(\mathbf{x}) - \rho_\gamma(\mathbf{x}))\, d\mathbf{x} \leq \int_{r<|\mathbf{x}|<r+s} \rho_r^{\rm OTF}(\mathbf{x}) V_r(\mathbf{x})\, d\mathbf{x} \leq Cr^{-8}s.$$

Choosing $s = r^{\frac{5}{3}}$ we find from (88) that

$$\mathcal{E}^A(\gamma_r^{\rm HF}) \leq \mathcal{E}^{\rm OTF}(\rho_r^{\rm OTF}) + Cr^{-7+\frac{2}{3}} + \mathcal{R}. \tag{89}$$

It remains to estimate $\mathcal{R}$. From Lemma 4.1, choosing $\lambda, \nu \leq 1/2$ and D such that $\sigma r^{\varepsilon'} \leq 1$ we find

$$\left(\tfrac{\pi}{2\lambda r} + \tfrac{C}{\lambda^2 r^2}\right) \int_{|\mathbf{x}| \geq r(1-\lambda)(1-\nu)} \rho^{\rm HF}(\mathbf{x})\, d\mathbf{x} \leq Cr^{-5}\lambda^{-2}.$$

By Lemma 4.8, (65) and since $\lambda \leq 1/2$ we get

$$\int_{r(1-\lambda) \leq |\mathbf{x}| \leq \frac{r}{1-\lambda}} (\Phi^{\rm HF}_{r(1-\lambda)}(\mathbf{x}))^{\frac{5}{2}}\, d\mathbf{x} \leq Cr^{-7}\lambda,$$

and similarly

$$\alpha^3 \int_{r(1-\lambda) \leq |\mathbf{x}| \leq \frac{r}{1-\lambda}} (\Phi^{\rm HF}_{r(1-\lambda)}(\mathbf{x}))^4\, d\mathbf{x} \leq Cr^{-4}\lambda,$$

since $r \geq \beta_0 Z^{-\frac{1}{3}}$ implies $\alpha r^{-3} \leq \beta_0^{-3}\kappa$. Hence from the expression of $\mathcal{R}$ and the boundness of $t^p e^{-t}$ for $t > 0$, we find

$$\mathcal{R} \leq \mathcal{E}x(\gamma_r^{\rm HF}) + Cr^{-5}\lambda^{-2} + Cr^{-7}\lambda. \tag{90}$$

We estimate now the exchange term. By the exchange inequality ([15] or [23, Th.6.4]) and proceeding as in (27) we find by Lemma 4.1 and Lemma 4.12

$$\begin{aligned}\mathcal{E}x(\gamma_r^{\mathrm{HF}}) &\leq C\int_{\mathbb{R}^3} G_\alpha(\rho_r^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x} + Cr^{-\frac{3}{2}}\Big(\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho_r^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x}\Big)^{\frac{1}{2}}\\ &\leq C\alpha\mathcal{R} + C\alpha r^{-7} + Cr^{-\frac{3}{2}}(\mathcal{R}+r^{-7})^{\frac{1}{2}}.\end{aligned}$$

Hence choosing α_0 such that $1 - C\alpha \geq 1/2$ for all $\alpha \leq \alpha_0$ we get from the inequality above and (90)

$$\tfrac{1}{2}\mathcal{R} \leq Cr^{-\frac{3}{2}}(\mathcal{R}+r^{-7})^{\frac{1}{2}} + Cr^{-5}\lambda^{-2} + Cr^{-7}\lambda\,,$$

that gives

$$\mathcal{R} \leq C(r^{-5}\lambda^{-2} + \lambda r^{-7})\,. \tag{91}$$

The second two inequalities in (84) follow from the estimate above and lemmas 4.1 and 4.12 choosing $\lambda = 1/2$ and replacing r with $r/2$.
Step II. Estimate from below on $\mathcal{E}^A(\gamma_r^{\mathrm{HF}})$. Adding and subtracting $D(\rho_r^{\mathrm{OTF}})$ and $\mathrm{Tr}[\rho_r^{\mathrm{OTF}} * \frac{1}{|\cdot|}\gamma_r^{\mathrm{HF}}]$ we write

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) = \mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}})\gamma_r^{\mathrm{HF}}] + \|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 - D(\rho_r^{\mathrm{OTF}}), \tag{92}$$

using that $V_r = \Phi_r^{\mathrm{HF}}$ on the support of ρ_r^{HF}. The first term on the right hand side of (92) is estimated from below by the sum of the first N' eigenvalues of the operator $\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}$ acting on the functions with support on $\{\mathbf{x} : |\mathbf{x}| \geq r\}$. Here N' denotes the smallest integer bigger than $\mathrm{Tr}[\gamma_r^{\mathrm{HF}}]$. Hence by Lemma 4.13 we find for $\mu \in (0,1)$ and $s < r$

$$\begin{aligned}\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \geq\; & -(\tfrac{2}{1-\mu})^{\frac{3}{2}}\tfrac{q}{15\pi^2}\int_{\mathbb{R}^3}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - Cr^{-8}s\mu^{-\frac{3}{2}} - C\mu^{-3}r^{-5}s\\ & -C(1-\mu)^{-\frac{7}{2}}r^{-5} - C(1-\mu)s^{-2}\Big(\int_{\mathbb{R}^3}\rho_r^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}+1\Big)\\ & +\|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 - D(\rho_r^{\mathrm{OTF}}) = \ldots,\end{aligned}$$

Notice the factor q due to spin. Choosing D such that $\sigma r^{\varepsilon'} \leq 1$, by lemmas 4.1 and 4.10 we find

$$\int_{\mathbb{R}^3}\rho_r^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} \leq Cr^{-3} \text{ and } \int_{\mathbb{R}^3}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} \leq Cr^{-7}.$$

Hence considering $\mu \leq 1/2$

$$\begin{aligned}\ldots \geq\; & -2^{\frac{3}{2}}\tfrac{q}{15\pi^2}\int_{\mathbb{R}^3}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - Cr^{-7} - Cr^{-8}s\mu^{-\frac{3}{2}} - C\mu^{-3}r^{-5}s\\ & -Cs^{-2}r^{-3} + \|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 - D(\rho_r^{\mathrm{OTF}}) = \ldots.\end{aligned}$$

By the OTF-equation (66) and since ρ_r^{OTF} has support where $\varphi_r^{\mathrm{OTF}} \geq 0$ we find

$$\cdots = \mathcal{E}^{\mathrm{OTF}}(\rho_r^{\mathrm{OTF}}) - Cr^{-7+\frac{1}{3}} + \|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2,$$

choosing $\mu = \frac{1}{2} r^{-\frac{2}{5}} s^{\frac{2}{5}}$ and $s = r^{\frac{11}{6}}$.
Hence combining the inequality above with (89) and (91) we find

$$\|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 \le C r^{-7+\frac{1}{3}} + C(r^{-5}\lambda^{-2} + \lambda r^{-7}). \tag{93}$$

We study now $\|\chi_r^+ \rho^{\mathrm{HF}} - \rho_r^{\mathrm{HF}}\|_C$. By Hardy-Littlewood-Sobolev inequality we find

$$\|\chi_r^+ \rho^{\mathrm{HF}} - \rho_r^{\mathrm{HF}}\|_C \le C\|\chi_r^+ \rho^{\mathrm{HF}} - \rho_r^{\mathrm{HF}}\|_{\frac{6}{5}} \le C\Big(\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}} \rho^{\mathrm{HF}}(\mathbf{x})^{\frac{6}{5}}\, d\mathbf{x}\Big)^{\frac{5}{6}}. \tag{94}$$

To estimate the last term in (94) we are going to use the second estimate in (84) that we have just proved. With Σ defined as in (26) we find by Hölder's inequality

$$\begin{aligned}
\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}} \rho^{\mathrm{HF}}(\mathbf{x})^{\frac{6}{5}}\, d\mathbf{x} \quad &\le \quad \Big(\int_{\substack{r\le|\mathbf{x}|,\\ \mathbf{x}\in\Sigma}} \rho^{\mathrm{HF}}(\mathbf{x})^{\frac{4}{3}}\, d\mathbf{x}\Big)^{\frac{9}{10}} \Big(\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}} 1\, d\mathbf{x}\Big)^{\frac{1}{10}} \\
&\quad + \Big(\int_{\substack{r\le|\mathbf{x}|,\\ \mathbf{x}\in\mathbb{R}^3\setminus\Sigma}} \rho^{\mathrm{HF}}(\mathbf{x})^{\frac{5}{3}}\, d\mathbf{x}\Big)^{\frac{18}{25}} \Big(\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}} 1\, d\mathbf{x}\Big)^{\frac{7}{25}} \\
&\le \quad C r^{-\frac{33}{10}}\lambda^{\frac{1}{10}} + C r^{-\frac{21}{5}}\lambda^{\frac{7}{25}}.
\end{aligned}$$

From the estimate above, (93) and (94) it then follows

$$\begin{aligned}
\|\chi_r^+ \rho^{\mathrm{HF}} - \rho_r^{\mathrm{OTF}}\|_C \quad &\le \quad \|\chi_r^+ \rho^{\mathrm{HF}} - \rho_r^{\mathrm{HF}}\|_C + \|\rho_r^{\mathrm{HF}} - \rho_r^{\mathrm{OTF}}\|_C \\
&\le C r^{-\frac{7}{2}+\frac{1}{6}} + C(r^{-5}\lambda^{-2} + \lambda r^{-7})^{\frac{1}{2}} + C(r^{-\frac{11}{4}}\lambda^{\frac{1}{12}} + r^{-\frac{7}{2}}\lambda^{\frac{7}{30}}),
\end{aligned}$$

that gives the claim choosing $\lambda = r^{\frac{5}{7}}$ □

4.3.3 Estimate on $\mathcal{A}_3$

Lemma 4.15. *Let G_α be the function defined in Theorem 2.3. Let $Z\alpha = \kappa$ fixed, $0 \le \kappa < 2/\pi$ and $Z \ge 1$.*
There exists $\alpha_0 > 0$ such that given $\varepsilon', \sigma > 0$ there exists a constant $D < 1/4$ depending only on ε' and σ such that if (64) *holds for all $|\mathbf{x}| \le D$, then for all $\alpha \le \alpha_0$*

$$\alpha^{-1}\int_{|\mathbf{y}|\ge|\mathbf{x}|} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y} \le C|\mathbf{x}|^{-7} \text{ for all } |\mathbf{x}| \le D,$$

with C a universal positive constant.

Proof. If $|\mathbf{x}| < \beta_0 Z^{-\frac{1}{3}}$ we find by Lemma 3.1

$$\alpha^{-1}\int_{|\mathbf{y}|>|\mathbf{x}|} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y} \le \alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y} \le C Z^{\frac{7}{3}} \le C|\mathbf{x}|^{-7}.$$

While if $D \ge |\mathbf{x}| \ge \beta_0 Z^{-\frac{1}{3}}$ the claim follows from the second estimate in (84). □

Lemma 4.16. *Let $Z\alpha = \kappa$ fixed, $0 \le \kappa < 2/\pi$, $Z \ge 1$ and $0 < \mu < \frac{1}{109}$. There exists α_0 such that given $\varepsilon', \sigma > 0$ there exists a constant $D < 1/4$ depending only on ε' and σ such that for all $\alpha \le \alpha_0$ and for all r with $\beta_0 Z^{-\frac{1-\mu}{3}} \le r \le D$ for which (64) holds for $|\mathbf{x}| \le r$, then for all $\mathbf{x}$ with $|\mathbf{x}| \ge r$*

$$|\mathcal{A}_3(r,\mathbf{x})| \le C\Big(\frac{|\mathbf{x}|}{r}\Big)^{\frac{1}{12}} r^{-4+\frac{3\mu}{1-\mu}},$$

with $C > 0$ a universal constant.

Proof. We proceed similarly as in Theorem 3.3. By the formula for $\mathcal{A}_3$, Proposition 2.8 and Lemma 4.14 we get

$$|\mathcal{A}_3(r,\mathbf{x})| \le \int_{A(|\mathbf{x}|,k)} \chi_r^+(\mathbf{y}) \frac{|\rho_r^{\mathrm{OTF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} + Ck^{-1}|\mathbf{x}|^{-\frac{1}{2}} r^{-\frac{7}{2}+\frac{1}{6}}. \quad (95)$$

By Hölder's inequality, Lemma 4.10, the OTF-equation (66) and (33) we find

$$\int_{A(|\mathbf{x}|,k)} \frac{\rho_r^{\mathrm{OTF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \le Cr^{-\frac{21}{5}}|\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}}. \quad (96)$$

Once again, to estimate $\int_{A(|\mathbf{x}|,k)} \frac{\chi_r^+(\mathbf{y})\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}$ we have to proceed differently than in [23, Lem.12.7] since ρ^{HF} is not in $L^{\frac{5}{3}}(\mathbb{R}^3)$. We consider the following splitting

$$\int_{A(|\mathbf{x}|,k)} \chi_r^+(\mathbf{y}) \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} = \int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R, |\mathbf{y}|>r}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} + \int_{\substack{|\mathbf{y}|>r,\\ |\mathbf{x}-\mathbf{y}|<R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}, \quad (97)$$

for $R > 0$ to be chosen. By Hölder's inequality, Theorem 2.3, Remark 2.4, (33) and Lemma 4.14 we get

$$\int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R, |\mathbf{y}|>r}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \le C\alpha^{\frac{3}{4}} R^{-\frac{3}{8}} |\mathbf{x}|^{\frac{1}{8}} k^{\frac{1}{8}} r^{-\frac{21}{4}} + Cr^{-\frac{21}{5}}|\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}}. \quad (98)$$

It remains to study the second term on the right hand side of (97). Let $\nu \in \mathbb{R}^+$ be such that $\nu\alpha \le 2/\pi$. We consider the density matrix $\gamma_{r/2}^{\mathrm{HF}}$ defined in (61) with $\lambda = 1/2$. From Theorem 2.10 it follows that for $\mathbf{x}$ such that $|\mathbf{x}| \ge r$

$$\mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - \frac{\nu}{|\cdot - \mathbf{x}|}\chi_{B_R(\mathbf{x})}(\cdot))\gamma_{r/2}^{\mathrm{HF}}] \ge -C(\nu^{\frac{5}{2}} R^{\frac{1}{2}} + \nu^4\alpha^2).$$

Hence we find

$$\begin{aligned}
\nu \int_{|\mathbf{y}-\mathbf{x}|<R} \chi_r^+(\mathbf{y}) \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \quad &\le \quad \nu \int_{|\mathbf{y}-\mathbf{x}|<R} \frac{\rho_{r/2}^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \\
&\le \quad \mathrm{Tr}[\alpha^{-1}T(\mathbf{p})\gamma_{r/2}^{\mathrm{HF}}] + C(\nu^{\frac{5}{2}} R^{\frac{1}{2}} + \nu^4\alpha^2)
\end{aligned}$$

and by Lemma 4.14

$$\int_{|\mathbf{y}-\mathbf{x}|<R} \chi_r^+(\mathbf{y}) \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \leq C\nu^{-1} r^{-7} + C(\nu^{\frac{3}{2}} R^{\frac{1}{2}} + \nu^3 \alpha^2). \tag{99}$$

Hence from (95), (96), (98) and (99) it follows that

$$\begin{aligned} |\mathcal{A}_3(r,\mathbf{x})| \leq\ & C\nu^{-1} r^{-7} + C(\nu^{\frac{3}{2}} R^{\frac{1}{2}} + \nu^3\alpha^2) + C\alpha^{\frac{3}{4}} R^{-\frac{3}{8}} |\mathbf{x}|^{\frac{1}{8}} k^{\frac{1}{8}} r^{-\frac{21}{4}} \\ & + Cr^{-\frac{21}{5}} |\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}} + Ck^{-1} |\mathbf{x}|^{-\frac{1}{2}} r^{-\frac{7}{2}+\frac{1}{6}}. \end{aligned}$$

So choosing $\nu = 1/2(\beta_0 r^{-1})^{\frac{3}{1-\mu}}$ (that gives $\nu\alpha < 2/\pi$), k such that $r^{-\frac{21}{5}}|\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}} = k^{-1}|\mathbf{x}|^{-\frac{1}{2}} r^{-\frac{7}{2}+\frac{1}{6}}$, i.e. $k = |\mathbf{x}|^{-\frac{7}{12}} r^{\frac{13}{18}}$ and R such that $\alpha^{\frac{3}{4}} R^{-\frac{3}{8}} |\mathbf{x}|^{\frac{1}{8}\frac{5}{12}} r^{-\frac{21}{4}+\frac{1}{8}\frac{13}{18}} = r^{-4-\frac{1}{18}} |\mathbf{x}|^{\frac{1}{12}}$, i.e. $R = \alpha^2 |\mathbf{x}|^{-\frac{1}{12}} r^{-\frac{5}{18}}$

$$|\mathcal{A}_3(r,\mathbf{x})| \leq C(r^{-4+\frac{3\mu}{1-\mu}} + |\mathbf{x}|^{-\frac{1}{24}} r^{-\frac{5}{36}-\frac{9}{2(1-\mu)}}\alpha + r^{-\frac{9}{1-\mu}}\alpha^2 + |\mathbf{x}|^{\frac{1}{12}} r^{-4-\frac{1}{18}}).$$

Finally since $r^{-1}\alpha^{\frac{1-\mu}{3}} \leq \beta_0^{-1}\kappa^{\frac{1-\mu}{3}}$, the claim follows for $|\mathbf{x}| \geq r$ and $\mu < 1/(109)$. ☐

4.4 The intermediate region

Here we prove the main estimate in Theorem 1.17 up to a fixed distance independent of Z.

Lemma 4.17 (Iterative step). *Let $Z\alpha = \kappa$ fixed with $0 \leq \kappa < 2/\pi$. Consider $\mu = \frac{1}{11}\frac{1}{49}$ and assume $N \geq Z \geq 1$.*
Then there exists $\alpha_0 > 0$ such that for all $\delta, \varepsilon', \sigma > 0$ with $\delta < \delta_0$, where δ_0 is some universal constant, there exists constants $\varepsilon_2, C'_\phi > 0$ depending only on δ and a constant $D = D(\varepsilon', \sigma) > 0$ depending only on ε', σ with the following property. For all $\alpha \leq \alpha_0$ and $R_0 < D$ satisfying that $\beta_0 Z^{-\frac{1-\mu}{3}} \leq R_0^{1+\delta}$ and that (64) holds for all $|\mathbf{x}| \leq R_0$, there exists $R'_0 > R_0$ such that

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C'_\Phi |\mathbf{x}|^{-4+\varepsilon_2}$$

for all $\mathbf{x}$ with $R_0 < |\mathbf{x}| < R'_0$.

Proof. Let $D > 0$ depending on σ, ε' be the smaller of the values of D occurring in Lemma 4.11 and Lemma 4.16. Given $\delta > 0$. We consider $R_0 < D$ satisfying $\beta_0 Z^{-\frac{1-\mu}{3}} \leq R_0^{1+\delta}$ and such that (64) holds for all $|\mathbf{x}| \leq R_0$.
Set $R'_0 = R_0^{1-\delta}$ and $r = R_0^{1+\delta}$. Then we have $\beta_0 Z^{-\frac{1}{3}} \leq \beta_0 Z^{-\frac{1-\mu}{3}} \leq r \leq R_0 < D$ we can therefore apply Lemma 4.11 and Lemma 4.16. From (67) we obtain that for all $|\mathbf{x}| \geq r$ and all $\alpha \leq \alpha_0$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C|\mathbf{x}|^{-4-\zeta} r^{\zeta} + C\Big(\frac{|\mathbf{x}|}{r}\Big)^{\frac{1}{12}} r^{-4+\frac{3\mu}{1-\mu}}.$$

Since for $R_0 < |\mathbf{x}| < R_0'$ we have

$$|\mathbf{x}|^{\frac{2\delta}{1-\delta}} \leq \frac{r}{|\mathbf{x}|} \leq |\mathbf{x}|^{\delta}$$

and thus

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C|\mathbf{x}|^{-4+\delta\zeta} + C|\mathbf{x}|^{-4+3\frac{\mu}{1-\mu}}|\mathbf{x}|^{-\frac{\delta}{1-\delta}(8+\frac{1}{6}-\frac{6\mu}{1-\mu})}.$$

Hence choosing δ_0 sufficiently small there are C'_Φ and ε_2 such that the claim holds. □

LEMMA 4.18. *Let $Z\alpha = \kappa$ fixed with $0 \leq \kappa < 2/\pi$. Assume $N \geq Z \geq 1$. Then there exist universal constants α_0, $\varepsilon \in (0,4)$ and $D, C_\Phi > 0$, $D < 1/4$, such that for all $\alpha \leq \alpha_0$ and $\mathbf{x}$ with $|\mathbf{x}| \leq D$ we have*

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C_\Phi |\mathbf{x}|^{-4+\varepsilon}.$$

Proof. We fix $\mu = \frac{1}{11}\frac{1}{49}$ as in Lemma 4.17. Since $\mu < \frac{2}{11}\frac{1}{49}$, by Theorem 3.3 we know that there exists constants $a, b, c > 0$ such that for all $|\mathbf{x}| \leq \beta Z^{-\frac{1-\mu}{3}}$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C(1 + \beta^2 + \beta^{5/2} + \beta^b|\mathbf{x}|^c)\beta^{2-a}|\mathbf{x}|^{-4+a}. \tag{100}$$

We first show that we may choose δ small enough such that if we choose $\tilde{R}^{1+\delta} = \beta_0 Z^{-\frac{1-\mu}{3}}$ we have for all $|\mathbf{x}| < \tilde{R}$ that

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C''_\Phi |\mathbf{x}|^{-4+\frac{a}{2}}. \tag{101}$$

Let $\beta > 0$ be such that $(\beta Z^{-\frac{1-\mu}{3}})^{1+\delta} = \beta_0 Z^{-\frac{1-\mu}{3}}$, i.e. $\beta^{1+\delta} = \beta_0 Z^{\delta\frac{1-\mu}{3}}$. Hence from (100) we find for all $|\mathbf{x}| \leq \beta Z^{-\frac{1-\mu}{3}}$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C(1 + \beta^2 + \beta^{5/2} + \beta^b|\mathbf{x}|^c)\beta^{2-\frac{a}{2}} Z^{-\frac{a}{2}\frac{1-\mu}{3}}|\mathbf{x}|^{-4+\frac{a}{2}},$$

and by the choice of β (and $\beta_0 < 1$)

$$\begin{aligned}|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \quad \leq \quad & C(1 + Z^{2\frac{\delta}{1+\delta}\frac{1-\mu}{3}} + Z^{\frac{5}{2}\frac{\delta}{1+\delta}\frac{1-\mu}{3}} + Z^{\frac{\delta}{1+\delta}\frac{1-\mu}{3}(b+c)}Z^{-c\frac{1-\mu}{3}}) \\ & Z^{(2-\frac{a}{2})\frac{1-\mu}{3}\frac{\delta}{1+\delta}} Z^{-\frac{a}{2}\frac{1-\mu}{3}}|\mathbf{x}|^{-4+\frac{a}{2}}.\end{aligned}$$

Hence if δ is small enough we may choose a universal constant C''_Φ such that (101) holds.
Let now δ be small enough so that we may apply Lemma 4.17. This give constant ε_2 and C'_Φ (depending only on δ) and for all $\sigma, \varepsilon' > 0$ a constant $D < 1/4$. Now choose $\sigma = \max\{C'_\Phi, C''_\Phi\}$ and $\varepsilon' = \min\{a/2, \varepsilon_2\}$. Now σ, ε' and D are universal constants. To prove the claim we shall prove that for all $|\mathbf{x}| \leq D$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq \sigma |\mathbf{x}|^{-4+\varepsilon'}. \tag{102}$$

We have to prove that D belongs to the set

$$\mathcal{M} = \{0 < R \leq 1/4 : \text{ Inequality (102) holds for all } |\mathbf{x}| \leq R\}.$$

We reason by contradiction. If this was not true then $D > R_0 = \sup \mathcal{M}$ and in particular $R_0 < 1/4$. From (101) and the choice of σ and ε' it follows that either $\tilde{R} > 1/4$ or $\tilde{R} \in \mathcal{M}$. In the first case then $R_0 = \sup \mathcal{M} = 1/4 > D$ that contradicts our hypothesis. On the other hand if $\tilde{R} \in \mathcal{M}$, then $R_0^{1+\delta} \geq \tilde{R}^{1+\delta} = \beta_0 Z^{-\frac{1-\mu}{3}}$. It then follows from Lemma 4.17 that there exists $R_0' \in \mathcal{M}$ with $R_0' > R_0$. This contradicts also our hypothesis. ☐

4.5 The outer zone and proof of Theorem 1.17

The proof of Theorem 1.17 follows directly from Lemma 4.18 and the following result.

Lemma 4.19. *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. Assume $N \geq Z \geq 1$. Let D, ε and C_Φ be the constants introduced in Lemma 4.18.*
Then there exist $\alpha_0 > 0$ and a universal constant $C_M > 0$ such that for all $\alpha \leq \alpha_0$ and $\mathbf{x}$ with $|\mathbf{x}| \geq D$ we have

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C_M.$$

Proof. Here C_i, $i = 1, \dots, 6$ denote positive universal constants. We write

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq |\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})| + \int_{D<|\mathbf{y}|<|\mathbf{x}|} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}. \tag{103}$$

Since $\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})$ is harmonic for $|\mathbf{x}| > D$ and tends to zero at infinity we have by Lemma 4.18

$$|\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})| \leq \sup_{|\mathbf{x}|=D} |\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})| \leq C_\phi D^{-4+\varepsilon}. \tag{104}$$

For the second term on the right hand side of (103) we write

$$\begin{aligned}
&\int_{D<|\mathbf{y}|<|\mathbf{x}|} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \\
&\leq \int_{\substack{|\mathbf{x}-\mathbf{y}|<D/4 \\ |\mathbf{y}|>D}} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} + \frac{4}{D} \int_{D<|\mathbf{y}|} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\, d\mathbf{y}.
\end{aligned} \tag{105}$$

By Lemma 4.1, Lemma 4.18, estimate (13) and the TF-equation we find

$$\int_{D<|\mathbf{y}|} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\, d\mathbf{y} \leq C_1(1 + C_\Phi D^{\varepsilon})(1 + D^{-3}) + C_1 D^{-3}. \tag{106}$$

It remains to estimate the first term on the right hand side of (105). By Hölder's inequality, estimate (13) and the TF-equation we get

$$\int_{\substack{|\mathbf{x}-\mathbf{y}|<D/4\\|\mathbf{y}|>D}} \frac{\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le C_2\Big(\int_{|\mathbf{y}|>D}(\rho^{\mathrm{TF}}(\mathbf{y}))^{\frac{5}{3}}\,d\mathbf{y}\Big)^{\frac{3}{5}} D^{\frac{1}{5}} \le C_3 D^{-4}. \quad (107)$$

To estimate the term with the HF-density we use Theorem 2.10. Let γ_D^{HF} be the exterior HF-density matrix as defined in (61) with $r = D/2$ and $\lambda = 1/2$. Then by Theorem 2.10 with $\nu = \beta_0^3 D^{-3}$

$$\alpha^{-1}\,\mathrm{Tr}[(T(\mathbf{p}) - \frac{\nu\alpha}{|\mathbf{x}-\cdot|}\chi_{B_{\frac{D}{4}}(\mathbf{x})}(\cdot))\gamma_{D/2}^{\mathrm{HF}}] \ge -C_4(D^{\frac{1}{2}}\nu^{\frac{5}{2}} + \nu^4\alpha^2),$$

and thus

$$\int_{|\mathbf{x}-\mathbf{y}|<D/4} \frac{\rho_{D/2}^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le C_5 D^3\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma_{D/2}^{\mathrm{HF}}] + C_6 D^{-4},$$

Here we use that $D > 2\beta_0 Z^{-\frac{1}{3}}$ (for $\alpha \le \alpha_0$) and $D < 1/4$. By Lemma 4.14 we conclude

$$\int_{|\mathbf{x}-\mathbf{y}|<D/4} \chi_D^+(\mathbf{y})\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le \int_{|\mathbf{x}-\mathbf{y}|<D/4} \frac{\rho_{D/2}^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le C_7 D^{-4}. \quad (108)$$

The claim follows collecting together formula (103) to formula (108). □

5 Proofs of Theorems 1.1, 1.18, 1.19 and 1.20

In this section we always assume the following: $Z\alpha = \kappa$ with $0 \le \kappa < 2/\pi$ and $N \ge Z \ge 1$.

Proof of Theorem 1.1. Assume that a HF-minimizer exists with $\int \rho^{\mathrm{HF}} = N$. Let ρ^{TF} be the minimizer of the TF-energy functional of the neutral atom with nuclear charge Z. Then for $R > 0$ to be chosen

$$N = \int_{|\mathbf{x}|<R} \rho^{\mathrm{TF}}(\mathbf{x})\,d\mathbf{x} + \int_{|\mathbf{x}|<R} (\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))\,d\mathbf{x} + \int_{|\mathbf{x}|>R} \rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}. \quad (109)$$

By Theorem 1.17 we know that there exist universal positive constants $\varepsilon, \alpha_0, C_M$ and C_Φ such that for all $\alpha \le \alpha_0$ and $\mathbf{x} \in \mathbb{R}^3$

$$|\Phi_{|\mathbf{x}|}^{\mathrm{HF}}(\mathbf{x}) - \Phi_{|\mathbf{x}|}^{\mathrm{TF}}(\mathbf{x})| \le C_\Phi|\mathbf{x}|^{-4+\varepsilon} + C_M. \quad (110)$$

Let Z_0 be such that $Z_0\alpha_0 = \kappa$. Then $\alpha \le \alpha_0$ corresponds to $Z \ge Z_0$. Let us choose R such that $C_\Phi R^{-4+\varepsilon} = C_M$. Then from (109), (110) and Lemma 4.1 for all $Z \ge Z_0$ we find

$$N \le \int_{|\mathbf{x}|<R} \rho^{\mathrm{TF}}(\mathbf{x})\,d\mathbf{x} + 2C_\Phi R^{-3+\varepsilon} + C(1 + C_\Phi R^{\varepsilon})(R^{-3}+1) < Z + \tilde{Q}.$$

The claim follows choosing $Q = \max\{\tilde{Q}, Z_0 + 1\}$. □

Proof of Theorem 1.18. Let ρ^{HF} be the density of the HF-minimizer in the neutral case $N = Z$. We have

$$\begin{aligned}\Big|\int_{|\mathbf{x}|>R}(\rho^{\mathrm{HF}}(\mathbf{x})-\rho^{\mathrm{TF}}(\mathbf{x}))d\mathbf{x}\Big| &= \Big|\int_{|\mathbf{x}|<R}(\rho^{\mathrm{HF}}(\mathbf{x})-\rho^{\mathrm{TF}}(\mathbf{x}))d\mathbf{x}\Big| \\ &= \Big|\frac{R}{4\pi}\int_{S^2}d\omega(\Phi_R^{\mathrm{HF}}(R\omega)-\Phi_R^{\mathrm{TF}}(R\omega))\Big| \\ &\le C_\Phi R^{-3+\varepsilon}+C_M R,\end{aligned}$$

where in the last step we have used Theorem 1.17. Notice that for Z sufficiently big $\alpha \le \alpha_0$ where α_0 is the constant given in Theorem 1.17. By the TF-equation, Theorem 1.12 we then find

$$\begin{aligned}3^4\frac{2\pi^2}{q^2}R^{-3}-C_\Phi R^{-3+\varepsilon}-C_M R &\le \int_{|\mathbf{x}|>R}\rho^{\mathrm{HF}}(\mathbf{x})d\mathbf{x} \\ &\le 3^4\frac{2\pi^2}{q^2}R^{-3}+C_\Phi R^{-3+\varepsilon}+C_M R,\end{aligned}$$

from which the claim follows directly by the definition of HF-radius. □

Proof of Theorem 1.19. Since $E^{\mathrm{HF}}(Z-1,Z) \ge E^{\mathrm{HF}}(Z,Z)$ the ionization energy is bounded from below by zero. If Z is smaller than a universal constant then we can also bound the ionization energy with a universal constant using Theorem 2.11.

It remains to estimate from above the ionization energy when Z is larger than a universal constant. We first construct a density matrix γ such that $\mathrm{Tr}[\gamma] \le Z-1$. Let $\theta_- := (1-\theta_{r(1-\lambda)}^2)^{\frac12}$ for r, λ positive parameters and θ_r defined in Definition 4.4. We consider the density matrix $\gamma_-^{\mathrm{HF}} := \theta_-\gamma^{\mathrm{HF}}\theta_-$ where γ^{HF} is the HF-minimizer in the neutral case. By an opportune choice of r we will then have $\mathrm{Tr}[\gamma_-^{\mathrm{HF}}] \le Z-1$. Indeed,

$$\mathrm{Tr}[\gamma_-^{\mathrm{HF}}] = \int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} - \int_{\mathbb{R}^3}\theta_{r(1-\lambda)}^2(\mathbf{x})\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} \le Z - \int_{|\mathbf{x}|>r}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}.$$

We now choose $\lambda = \frac12$. Let $R > 0$ be such that $C_M = C_\Phi R^{-4+\varepsilon}$ where C_M, C_Φ, ε are the constants in Theorem 1.17. Then R is a universal constant. We consider Z large enough so that $\beta_0 Z^{-\frac13} < R$ where β_0 is the constant in Theorem 1.12. This gives that Z has to be larger than some universal constant. For r such that $\beta_0 Z^{-\frac13} < r < R$ by Theorem 1.17 we find

$$|\Phi_{|\mathbf{x}|}^{\mathrm{HF}}(\mathbf{x}) - \Phi_{|\mathbf{x}|}^{\mathrm{TF}}(\mathbf{x})| \le 2C_\Phi|\mathbf{x}|^{-4+\varepsilon} \text{ for all } |\mathbf{x}| \le r.$$

Since $\int\rho^{\mathrm{TF}} = \int\rho^{\mathrm{HF}}$, by the choice of r and Lemma 4.1 we get

$$\begin{aligned}\int_{|\mathbf{x}|>r}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} &= \int_{|\mathbf{x}|>r}\rho^{\mathrm{TF}}(\mathbf{x})\,d\mathbf{x}+\int_{|\mathbf{x}|<r}(\rho^{\mathrm{TF}}(\mathbf{x})-\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} \\ &\ge \int_{|\mathbf{x}|>r}\rho^{\mathrm{TF}}(\mathbf{x})\,d\mathbf{x} - 2C_\Phi r^{-3+\varepsilon} \ge Cr^{-3}-2C_\Phi r^{-3+\varepsilon}. \quad (111)\end{aligned}$$

In the last step we used the TF-equation, Corollary 1.13 and that $r > \beta_0 Z^{-\frac{1}{3}}$. Finally, it follows from (111) by choosing r sufficiently small that $\int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}} > 1$ and hence that $\mathrm{Tr}[\gamma_-^{\mathrm{HF}}] \le Z-1$. We may choose r sufficiently small by taking Z large enough. Notice that r can be chosen universally and so Z has to be larger than some universal constant.

By the last estimate in the proof of Theorem 4.7 we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) \le \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) - \mathcal{E}^A(\gamma_r^{\mathrm{HF}}) + \mathcal{R},$$

with $\mathcal{R}$ and γ_r^{HF} as defined in the statement of Theorem 4.7. Since $\mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) \ge E^{\mathrm{HF}}(Z-1, Z)$ and $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = E^{\mathrm{HF}}(Z,Z)$ it remains to prove that $-\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) + \mathcal{R}$ is bounded from above by some universal constant. Here we use repeteadly that r is a universal constant. By estimate (91) we see that $\mathcal{R} \le Cr^{-7}$ a universal constant. To estimate from below $\mathcal{E}^A(\gamma_r^{\mathrm{HF}})$ we first leave out the kinetic energy term and the direct term since these are positive. Moreover, since Φ_r^{HF} is harmonic for $|\mathbf{x}| > r$ and tends to zero at infinity we see that

$$\Phi_r^{\mathrm{HF}}(\mathbf{x}) \le \frac{r}{|\mathbf{x}|} \sup_{|\mathbf{y}|=r} \Phi_r^{\mathrm{HF}}(\mathbf{y}) \le \frac{r}{|\mathbf{x}|} \sup_{|\mathbf{y}|=r} \Phi_r^{\mathrm{TF}}(\mathbf{y}) + \frac{r}{|\mathbf{x}|} \sup_{|\mathbf{y}|=r} |\Phi_r^{\mathrm{TF}}(\mathbf{y}) - \Phi_r^{\mathrm{HF}}(\mathbf{y})|,$$

which is bounded by $C'/|\mathbf{x}|$, C' a universal constant, by Theorem 1.17 and Corollary 1.14. It then follows that

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \ge -\mathrm{Tr}[\frac{C'}{|\cdot|}\gamma_r^{\mathrm{HF}}] \ge -\frac{C'}{r}\int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x},$$

that is bounded from below by a universal constant using Lemma 4.1. □

Proof of Theorem 1.20. Let α_0 be the constant appearing in Theorem 1.17 and Z_0 be such that $\alpha_0 Z_0 = \kappa$. The claim follows directly for $Z \le Z_0$ since both functions are bounded for $|\mathbf{x}|$ large, while for $|\mathbf{x}|$ small the functions are bounded by a constant times $|\mathbf{x}|^{-1}$.

The case $Z > Z_0$ corresponds to $\alpha < \alpha_0$ and for such values of α we can use the result in Theorem 1.17. We separate the case small $\mathbf{x}$, intermediate $\mathbf{x}$ and large $\mathbf{x}$. Once again, comparing with the proof in the non-relativistic case ([23]) we have to do an extra splitting for small $\mathbf{x}$.

By the definition of the mean field potential and Proposition 2.8 we find

$$\begin{aligned} |\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \quad &\le \quad \int_{|\mathbf{x}-\mathbf{y}|<s} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{s}\Big) \\ &\quad + \frac{\sqrt{2}}{s^{\frac{1}{2}}}\|\rho^{\mathrm{TF}} - \rho^{\mathrm{HF}}\|_C. \end{aligned}$$

Since ρ^{TF} is bounded in $L^{\frac{5}{3}}$-norm, we find using Hölder's inequality, Corollary 1.15 and Lemma 3.1 that

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \le \int_{|\mathbf{x}-\mathbf{y}|<s} \rho^{\mathrm{HF}}(\mathbf{y})\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{s}\Big) + C(s^{\frac{1}{5}} Z^{\frac{7}{5}} + s^{-\frac{1}{2}} Z^{1+\frac{3}{22}}). \tag{112}$$

For the integral with the HF-density we need to split the region where the HF-density is bounded in $L^{\frac{4}{3}}$-norm from the one where it is bounded in $L^{\frac{5}{3}}$-norm. Proceeding as in the proof of Lemma 3.2 (from (35) to (37) replacing the integrals on $A(|\mathbf{x}|,k)$ with integrals on $|\mathbf{x}-\mathbf{y}|<s$) using the results of Lemma 3.1 we get with $R\in(0,s)$ to be chosen

$$\int_{|\mathbf{x}-\mathbf{y}|<s}\rho^{\mathrm{HF}}(\mathbf{y})\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|}-\frac{1}{s}\Big)\le C(Z^{\frac{7}{5}}s^{\frac{1}{5}}+R^{-\frac{1}{4}}(\alpha Z^{\frac{7}{3}})^{\frac{3}{4}}+Z^{\frac{4}{3}}+R^{\frac{1}{2}}Z^{\frac{3}{2}}). \quad (113)$$

Recall that $Z\alpha=\kappa$ is fixed. Choosing s such that $Z^{\frac{7}{5}}s^{\frac{1}{5}}=Z^{\frac{4}{3}}$ (i.e. $s=Z^{-\frac{1}{3}}$) and R such that $R^{-\frac{1}{4}}Z=R^{\frac{1}{2}}Z^{\frac{3}{2}}$ (i.e $R=Z^{-\frac{2}{3}}$; notice that $R<s$) we get from (112) and (113)

$$|\varphi^{\mathrm{TF}}(\mathbf{x})-\varphi^{\mathrm{HF}}(\mathbf{x})|\le C(Z^{\frac{4}{3}}+Z^{\frac{7}{6}}).$$

The claim follows from this inequality for $\mathbf{x}\in\mathbb{R}^3$ such that $|\mathbf{x}|\le\beta_0Z^{-\frac{1+\gamma}{3}}$ for $\gamma>0$. We consider $\gamma<\frac{1}{263}$.

If $|\mathbf{x}|\ge\beta_0Z^{-\frac{1+\gamma}{3}}$ then proceeding as for very small $\mathbf{x}$ and as in the proof of Theorem 3.3 up to inequality (43) we get for $t\in(\frac{1+\gamma}{3},\frac{3}{5})$, $l>t$ and $R<\beta_0Z^{-l}$

$$|\varphi^{\mathrm{TF}}(\mathbf{x})-\varphi^{\mathrm{HF}}(\mathbf{x})|\le C(s^{\frac{1}{5}}Z^{\frac{7}{5}}+s^{-\frac{1}{2}}Z^{1+\frac{3}{22}}+R^{-\frac{3}{8}}s^{\frac{1}{8}}Z+Z^{\frac{1}{2}(3-t)}).$$

Here we have also used that $Z\alpha$ is a constant. So choosing s such that $s^{\frac{1}{5}}Z^{\frac{7}{5}}=Z^{\frac{1}{2}(3-t)}$ (i.e. $s=Z^{\frac{1}{2}-\frac{5}{2}t}$), R such that $R^{-\frac{3}{8}}Z^{1+\frac{1}{16}-\frac{5}{16}t}=Z^{\frac{1}{2}(3-t)}$ (i.e. $R=Z^{-\frac{7}{6}+\frac{1}{2}t}$) and optimizing in t (i.e. $t=\frac{1}{3}+\frac{4}{3}\frac{1}{77}$) we obtain

$$|\varphi^{\mathrm{TF}}(\mathbf{x})-\varphi^{\mathrm{HF}}(\mathbf{x})|\le CZ^{\frac{4}{3}-\frac{2}{3}\frac{1}{77}}. \quad (114)$$

Notice that $t>\frac{1+\gamma}{3}$, $R<s$ by the choice of t and that R satisfies the condition $R<\beta_0Z^{-l}$, $l>t$, for Z sufficiently big. The claim then follows from (114) for $\mathbf{x}\in\mathbb{R}^3$ such that $|\mathbf{x}|^{1+\delta}\le\beta_0Z^{-\frac{1}{3}}$ for $\delta<\frac{1}{153}$. We fix $\delta=\frac{1}{2}\frac{1}{153}$.

We turn now to study intermediate $\mathbf{x}$. Let $D\le1$ be such that $C_M\le C_\Phi D^{-4+\varepsilon}$ with C_M,C_Φ,ε the constants in Theorem 1.17. Then for all $\mathbf{x}$ such that $|\mathbf{x}|\le D$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})-\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})|\le 2C_\Phi|\mathbf{x}|^{-4+\varepsilon}.$$

Moreover we choose D such that Lemma 4.11 holds. Let $\mathbf{x}$ be such that $\beta_0Z^{-\frac{1}{3}}\le|\mathbf{x}|^{1+\delta}\le D^{\frac{1+\delta}{1+\mu}}$ with $0<\mu\le\delta$. We set $r=|\mathbf{x}|^{1+\mu}$. Then $\beta_0Z^{-\frac{1}{3}}\le r\le D$. We write $\varphi^{\mathrm{TF}}(\mathbf{x})-\varphi^{\mathrm{HF}}(\mathbf{x})=\varphi^{\mathrm{TF}}(\mathbf{x})-\varphi^{\mathrm{OTF}}_r(\mathbf{x})+\varphi^{\mathrm{OTF}}_r(\mathbf{x})-\varphi^{\mathrm{HF}}(\mathbf{x})$ with φ^{OTF}_r the mean field potential of the OTF-problem defined in Subsection 4.3. By the choice of r and D and Lemma 4.11 we get since $|\mathbf{x}|\ge r=|\mathbf{x}|^{1+\mu}$

$$|\varphi^{\mathrm{TF}}(\mathbf{x})-\varphi^{\mathrm{OTF}}_r(\mathbf{x})|\le C|\mathbf{x}|^{-4-\zeta}r^{\zeta}\,, \quad (115)$$

for $|\mathbf{x}|\ge r$ with $\zeta=(7+\sqrt{73})/2$. For the other two terms we see

$$\varphi^{\mathrm{HF}}(\mathbf{x})-\varphi^{\mathrm{OTF}}_r(\mathbf{x})=\int\frac{\rho^{\mathrm{OTF}}_r(\mathbf{y})-\chi^+_r(\mathbf{y})\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y},$$

and proceeding as for small $\mathbf{x}$ with the Coulomb-norm estimate Proposition 2.8, by Lemma 4.14 and inequality (99)

$$|\varphi^{\mathrm{HF}}(\mathbf{x})-\varphi_r^{\mathrm{OTF}}(\mathbf{x})| \le C\Big(\frac{s^{\frac{1}{5}}}{r^{\frac{21}{5}}}+\frac{r^{-\frac{7}{2}+\frac{1}{6}}}{s^{\frac{1}{2}}}+R^{-\frac{1}{4}}(\alpha r^{-7})^{\frac{3}{4}}+\nu^{-1}r^{-7}+\nu^{\frac{3}{2}}R^{\frac{1}{2}}+\nu^3\alpha^2\Big).$$

Choosing $\nu = \beta_0^3 r^{-3\frac{1+\delta}{1+\mu}}$, so that $\nu\alpha \le \kappa < 2/\pi$, s such that $s^{\frac{1}{5}}r^{-\frac{21}{5}} = r^{-\frac{7}{2}+\frac{1}{6}}s^{-\frac{1}{2}}$ (i.e. $s = r^{1+\frac{5}{21}}$), and choosing R such that the two terms where it appears are equal (i.e. $R = r^{2+9\frac{\delta-\mu}{1+\mu}}$; notice that $R < s$) we get

$$|\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi_r^{\mathrm{OTF}}(\mathbf{x})| \le C(r^{-4+\frac{1}{21}} + r^{-4+3\frac{\delta-\mu}{1+\mu}}),$$

since $\alpha r^{-3\frac{1+\delta}{1+\mu}}$ is bounded and $r \le 1$. Collecting together the inequality above and (115) and using that $r = |\mathbf{x}|^{1+\mu}$ the claim follows for $\beta_0 Z^{-\frac{1}{3}} \le |\mathbf{x}|^{1+\delta} \le D^{\frac{1+\delta}{1+\mu}}$. We fix $\mu = \delta/2$.

It remains to study the case of large $\mathbf{x}$, i.e. $|\mathbf{x}| \ge D^{\frac{1+\delta}{1+\mu}}$ with D, δ, μ universal constants. For simplicity of notation we fix the universal constant $A := D^{\frac{1+\delta}{1+\mu}}$. We first notice that

$$\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi^{\mathrm{TF}}(\mathbf{x}) = \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) + \int_{|\mathbf{y}|>|\mathbf{x}|} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}.$$

The difference of the first two terms is bounded by a universal constant for $|\mathbf{x}| \ge A$ by the result in Theorem 1.17. To estimate the last integral we split it as follows

$$\begin{aligned}\int_{|\mathbf{y}|>|\mathbf{x}|} \frac{|\rho^{\mathrm{TF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \quad &\le \quad \int_{\substack{|\mathbf{y}|>|\mathbf{x}|\\|\mathbf{x}-\mathbf{y}|<1}} \frac{\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} + \int_{\substack{|\mathbf{y}|>|\mathbf{x}|\\|\mathbf{x}-\mathbf{y}|<1}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}\\ &\quad + \int_{|\mathbf{y}|>|\mathbf{x}|} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\, d\mathbf{y}.\end{aligned}$$

Since $|\mathbf{x}| \ge A$ the third term on the right hand side is bounded by a universal constant by Lemma 4.1 (for ρ^{HF}) and Corollary 1.13 (for ρ^{TF}). We estimate the first term by Hölder's inequality and Corollary 1.15. We get a bound on the second term proceeding as in (99) (using Theorem 2.10) and choosing $\nu = \frac{1}{2}$ and $R = 1$. We obtain

$$\int_{\substack{|\mathbf{y}|>|\mathbf{x}|\\|\mathbf{x}-\mathbf{y}|<1}} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \le C(A^{-\frac{21}{5}} + A^{-7} + \alpha^2).$$

Then there exists a universal contant A' such that $|\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi^{\mathrm{TF}}(\mathbf{x})| \le A'$ for $|\mathbf{x}| \ge A$. □

A Technical lemmas

PROOF OF (16) By the definition of the function G_α the inequalities in (16) are equivalent to the following ones

$$\tfrac{3}{5}t^4 \min\{\tfrac{2}{5}t, 1\} \leq g(t) - \tfrac{8}{3}t^3 \leq 2t^4 \min\{\tfrac{2}{5}t, 1\} \text{ for } t \geq 0. \tag{A1}$$

As before we use the substitution $t = \alpha(\rho/C)^{\frac{1}{3}}$.
The estimates in (A1) follow directly from the study of the function g separating the cases $t < \frac{5}{2}$ and $t \geq \frac{5}{2}$.
PROOF OF REMARK 4.2 Using the estimate on K_2 given in (15) we find

$$\begin{aligned}
&\iint_{\substack{\mathbf{x} \in \Sigma_r(\beta_1, \beta_2) \\ \mathbf{y} \in \Sigma_r(\beta_3, \beta_4)}} K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|)^2 \, d\mathbf{x}d\mathbf{y} \\
\leq \;& (16)^2\alpha^4 \iint_{\substack{\mathbf{x} \in \Sigma_r(\beta_1, \beta_2) \\ \mathbf{y} \in \Sigma_r(\beta_3, \beta_4)}} \frac{e^{-\alpha^{-1}|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x} - \mathbf{y}|^4} \, d\mathbf{x}d\mathbf{y} \\
\leq \;& (16)^2\alpha^4 e^{-\alpha^{-1}r(\beta_3-\beta_2)} 4\pi \int_{r(\beta_3-\beta_2)}^{\infty} \rho^{-2} d\rho \int_{\Sigma_r(\beta_1,\beta_2)} d\mathbf{x},
\end{aligned}$$

since $|\mathbf{x} - \mathbf{y}| \geq (\beta_3 - \beta_2)r$. The claim follows computing the two integrals.

A.1 Fourier transform

In the present sub-section we present our notation for the Fourier transform (as in [20]). Given $f \in L^2(\mathbb{R}^3)$ we denote its Fourier transform by

$$\hat{f}(\mathbf{p}) = \mathcal{F}(f)(\mathbf{p}) := \tfrac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} e^{i\mathbf{p}\cdot x} f(\mathbf{x}) d\mathbf{x}.$$

Let $f, g \in L^2(\mathbb{R}^3)$. The following formulas hold:

1. $\mathcal{F}(f * g)(\mathbf{p}) = (2\pi)^{\frac{3}{2}} \hat{f}(\mathbf{p})\hat{g}(\mathbf{p})$;
2. $\mathcal{F}(fg)(\mathbf{p}) = (2\pi)^{-\frac{3}{2}} (\hat{f} * \hat{g})(\mathbf{p})$;
3. if $g(\mathbf{x}) = e^{-\lambda|\mathbf{x}|^2}$ then $\hat{g}(\mathbf{p}) = (2\lambda)^{-\frac{3}{2}} e^{-|\mathbf{p}|^2/(4\lambda)}$;
4. $|\mathbf{x}|^{-\alpha} = \pi^{\frac{\alpha}{2}} (\Gamma(\frac{\alpha}{2}))^{-1} \int_0^{+\infty} e^{-\pi|\mathbf{x}|^2\lambda} \lambda^{\frac{\alpha}{2}-1} d\lambda$ for $0 < \alpha < n$ (see [14, page 130]).

Moreover,

$$\mathcal{F}\Big(\frac{f(\mathbf{x})}{|\mathbf{x}|}\Big)(\mathbf{k}) = \tfrac{1}{2\pi^2} \int_{\mathbb{R}^3} \frac{\hat{f}(\mathbf{p})}{|\mathbf{k} - \mathbf{p}|^2} d\mathbf{p}.$$

B Large Z-behavior of the energy

In [21] the author studies the large Z-behavior of the ground state energy for problem (1). In this work we are going to use the same construction in several points (Lemmas 3.1, 4.12, Theorem 3.3, ...) and with, in certain cases, a slightly different Hamiltonian. For convenience we repeat here the main ideas of the proof. We do it as it is needed in the proof of Theorem 3.3 since in this case the proof is more involved. We remark that in our proof we use a localisation less than in [21]. Thanks to Theorem 2.10 and [24, Theorem 2.8] it is sufficient to consider the region near the nuclei and the one far away from the nuclei. There is no need for an intermediate region.

Proposition B.1. *Let $Z\alpha = \kappa$ be fixed with $0 \le \kappa < 2/\pi$ and $Z \ge 1$. Let us consider $\mathbf{P} \in \mathbb{R}^3$, with $|\mathbf{P}| \ge \beta Z^{-\frac{1+\mu}{3}}$ for $\beta > 0$ and $\mu \in (0, 4/5)$. Let $Z \ge \nu > 0$ and $R > 0$ be such that $R < \beta Z^{-l}/4$ for some $\frac{1+\mu}{3} < l$. Moreover, let ρ^{TF} denote the minimizer of the TF-energy functional of a neutral atom with nucleus of charge Z. Consider the Hamiltonian*

$$H_{\mathbf{P}} := \sum_{i=1}^{N} \left(\alpha^{-1} T(\mathbf{p}_i) - \frac{Z}{|\mathbf{x}_i|} - \frac{\nu}{|\mathbf{x}_i - \mathbf{P}|}\chi_{B_R(\mathbf{P})}(\mathbf{x}_i)\right) + \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \qquad \text{(B2)}$$

acting on $\wedge_{i=1}^{N} L^2(\mathbb{R}^3; \mathbb{C}^q)$.
Then for all $t \in (\frac{1+\mu}{3}, \min\{l, \frac{3}{5}\})$ and $\psi \in \wedge_{i=1}^{N} L^2(\mathbb{R}^3)$, with $\|\psi\|_2 = 1$,

$$\langle \psi, H_{\mathbf{p}} \psi \rangle \ge \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - C(\beta^{\frac{1}{2}} + \beta^{-2}) Z^{\frac{5}{2} - \frac{1}{2}t},$$

with C depending only on q and κ.

Proof. Since $\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = -e_0 Z^{\frac{7}{3}}$ (see (12)) to prove the claim it is sufficient to show that the TF-energy gives a lower bound to the quantum energy modulo lower order terms. In the proof we first reduce to a one-particle operator. Then we localize the energy separating the contribution from the regions near the nuclei from the contribution from the region far away from them. Finally we study the contribution of each of these terms. The main contribution to the energy is given by the region far away from the nuclei. This region will give the TF-energy.
In the following, $s = (3 - t)/4$ ($t < s < 2/3$).
In the proof C denotes a generic positive constant depending only on q and κ.
Reduction to a one-particle problem. We are going to estimate from below $H_{\mathbf{P}}$ by a one-particle operator. This allows us to consider only Slater determinants when minimizing the energy.
Let $g \in C_0^\infty(\mathbb{R}^3)$, $g \ge 0$ be spherically symmetric with $\mathrm{supp}(g) \subset B_1(0)$ and such that $\|g\|_2 = 1$. Starting from these g we define $\Phi_s(\mathbf{x}) :=$

$(\beta/(8Z^s))^{-3}g^2(8Z^s\mathbf{x}/\beta)$. Then by Newton's theorem

$$\sum_{i<j}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\geq\sum_{i<j}\iint\frac{\Phi_s(\mathbf{x}_i-\mathbf{x})\Phi_s(\mathbf{x}_j-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}=$$

$$=\ \tfrac{1}{2}\sum_{i,j=1}^{N}\iint\frac{\Phi_s(\mathbf{x}_i-\mathbf{x})\Phi_s(\mathbf{x}_j-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}-\tfrac{N}{2}\iint\frac{\Phi_s(\mathbf{x})\Phi_s(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}=\dots$$

and introducing $\rho\in L^1(\mathbb{R}^3)\cap L^{\frac{5}{3}}(\mathbb{R}^3)$, $\rho\geq 0$, to be chosen

$$\begin{aligned}\dots\ &=\ \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{(\sum_{i=1}^{N}\Phi_s(\mathbf{x}_i-\mathbf{x})-\rho(\mathbf{x}))(\sum_{j=1}^{N}\Phi_s(\mathbf{x}_j-\mathbf{y})-\rho(\mathbf{y}))}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\\ &+\ \sum_{i=1}^{N}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\Phi_s(\mathbf{x}_i-\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}-D(\rho)-\tfrac{N}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\Phi_s(\mathbf{x})\Phi_s(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\\ &\geq\ \sum_{i=1}^{N}\rho*\Phi_s*\frac{1}{|\mathbf{x}_i|}-D(\rho)-C\|g^2\|_{\frac{6}{5}}^2N\beta^{-1}Z^s.\end{aligned}\tag{B3}$$

In the last inequality we use that the first term on the left hand side of (B3) is non-negative and that

$$\begin{aligned}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\Phi_s(\mathbf{x})\Phi_s(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\ &=\ C\beta^{-1}Z^s\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{g^2(\mathbf{x})g^2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\\ &\leq\ C\beta^{-1}Z^s\|g^2\|_{6/5}^2,\end{aligned}$$

by definition of Φ_s and Hardy-Littlewood-Sobolev's inequality. Hence

$$\begin{aligned}H_{\mathbf{P}}\ \geq\ &\sum_{i=1}^{N}\big(\alpha^{-1}T(\mathbf{p}_i)-\frac{Z}{|\mathbf{x}_i|}-\frac{\nu}{|\mathbf{x}_i-\mathbf{P}|}\chi_{B_R(\mathbf{P})}(\mathbf{x}_i)+\rho*\Phi_s*\frac{1}{|\mathbf{x}_i|}\big)\\ &-D(\rho)-C\|g^2\|_{\frac{6}{5}}^2N\beta^{-1}Z^s.\end{aligned}\tag{B4}$$

Choice of the localization. The localization will be given by the following functions $\chi_1,\chi_2\in C_0^\infty(\mathbb{R}^3)$:

$$\chi_1(\mathbf{x}):=\begin{cases}1 & \text{if } |\mathbf{x}|<\frac{1}{4}\beta Z^{-t},\\ 0 & \text{if } |\mathbf{x}|>\frac{1}{2}\beta Z^{-t},\end{cases}\quad \chi_2(\mathbf{x}):=\begin{cases}1 & \text{if } |\mathbf{x}-\mathbf{P}|<\frac{1}{4}\beta Z^{-t},\\ 0 & \text{if } |\mathbf{x}-\mathbf{P}|>\frac{1}{2}\beta Z^{-t}\end{cases}\tag{B5}$$

and $\chi_3\in C^\infty(\mathbb{R}^3)$ such that $\sum_{i=1}^{3}\chi_i^2(\mathbf{x})=1$ for all $\mathbf{x}\in\mathbb{R}^3$. Moreover we ask that

$$\|\nabla\chi_1\|_\infty,\|\nabla\chi_2\|_\infty,\|\nabla\chi_3\|_\infty\leq 2^5\beta^{-1}Z^t.\tag{B6}$$

Here t is the parameter given in the statement of the proposition. Notice that by the assumptions on R and $\mathbf{P}$ the functions defined above give a well defined partition of unity of $\mathbb{R}^3$. Moreover, $B_R(\mathbf{P})$ is a subset of $\{\mathbf{x}\in\mathbb{R}^3:\chi_2(\mathbf{x})=1\}$.

The localization in the energy expectation. We insert now the localization in the energy expectation. As already observed, since we reduced the operator to a one-particle operator in the energy expectation it is sufficient to consider Slater determinants: i.e. $\psi = u_1 \wedge \cdots \wedge u_N$ with $\{u_i\}_{i=1}^N$ orthonormal functions in $L^2(\mathbb{R}^3, \mathbb{C}^q)$. We may assume that $u_i \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$ for $i = 1, \ldots, N$.
From (B4) and Theorem 2.1 we find with $\psi = u_1 \wedge \cdots \wedge u_N$

$$\begin{aligned}\langle \psi, H_{\mathbf{P}} \psi \rangle \quad \geq \quad & \sum_{i=1}^N \sum_{j=1}^3 (\chi_j u_i, h \chi_j u_i) - D(\rho) - C \|g^2\|_{\frac{6}{5}}^2 N \beta^{-1} Z^s \\ & -\alpha^{-1} \sum_{i=1}^N \sum_{j=1}^3 (u_i, L_j u_i), \end{aligned} \tag{B7}$$

with

$$h := \alpha^{-1} T(\mathbf{p}) - \frac{Z}{|\cdot|} - \frac{\nu \, \chi_{B_R(\mathbf{P})}(\cdot)}{|\cdot - \mathbf{P}|} + \rho * \Phi_s * \frac{1}{|\cdot|},$$

and L_j is the operator (defined in Theorem 2.1) that gives the error due to the localization in the kinetic energy. We first estimate this error term. Using the definition of L_j we find for all $j \in \{1, 2, 3\}$, $i \in \{1, \ldots, N\}$

$$(u_i, L_j u_i) \leq \frac{\alpha^{-2}}{4\pi^2} \|\nabla \chi_j\|_\infty^2 \iint K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|) |u_i(\mathbf{y})| |u_i(\mathbf{x})| \, d\mathbf{x} d\mathbf{y}.$$

We then obtain by using Schwarz's inequality

$$\alpha^{-1} \sum_{i=1}^N \sum_{j=1}^3 (u_i, L_j u_i) \leq \frac{\alpha^{-3}}{4\pi^2} \sum_{j=1}^3 \|\nabla \chi_j\|_\infty^2 \sum_{i=1}^N \int K_2(\alpha^{-1}|\mathbf{z}|) d\mathbf{z} \leq C N \beta^{-2} Z^{2t}, \tag{B8}$$

since from (15)

$$\int_{\mathbb{R}^3} K_2(\alpha^{-1}|\mathbf{z}|) \, d\mathbf{z} = \alpha^3 \int_{\mathbb{R}^3} K_2(|\mathbf{z}|) \, d\mathbf{z} = 4\pi \alpha^3 \int_0^\infty t^2 K_2(t) \, dt = 6\pi^2 \alpha^3. \tag{B9}$$

Collecting together (B7) and (B8) we get

$$\langle \psi, H_{\mathbf{P}} \psi \rangle \geq \sum_{i=1}^N \sum_{j=1}^3 (\chi_j u_i, h \chi_j u_i) - D(\rho) - C \beta^{-2} Z^{1+2t} - C \beta^{-1} Z^{7/4 - t/4}. \tag{B10}$$

Here we used that $N \leq 2Z + 1$, the choice of s and that we may choose g such that $\|\nabla g\|_2^2 \leq 2\pi$.
Near the nuclei. When $j = 1$ in the summation in the first term on the right hand side of (B10) we find

$$\sum_{i=1}^N (\chi_1 u_i, h \chi_1 u_i) \geq \sum_{i=1}^N (\chi_1 u_i, (\alpha^{-1} T(\mathbf{p}) - \frac{Z}{|\cdot|}) \chi_1 u_i),$$

since $\chi_{B_R(\mathbf{P})}\chi_1 \equiv 0$ by the choice of χ_1, and the term $\Phi_s * \rho * \frac{1}{|\cdot|}$ is non-negative. Then by Theorem 2.10 we find

$$\begin{aligned}\sum_{i=1}^{N}(\chi_1 u_i, h\chi_1 u_i) &\geq \operatorname{Tr}[\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\cdot|}\chi_{|\mathbf{x}|<\frac{1}{2}\beta Z^{-t}}]_- \\ &\geq -C\beta^{1/2}Z^{5/2-t/2} - C\kappa^2 Z^2. \qquad \text{(B11)}\end{aligned}$$

To estimate from below the term corresponding to $j = 2$ in the sum on the right hand side of (B10) we use [24, Theorem 2.8]. Here we need the result in [24] (instead of Theorem 2.10) because of the presence of the two nuclei. Notice that Theorem 2.10 can be extended to include also different nuclei. We have

$$\begin{aligned}\sum_{i=1}^{N}(\chi_2 u_i, h\chi_2 u_i) &\geq \sum_{i=1}^{N}(\chi_2 u_i, (\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\mathbf{x}|} - \frac{\nu}{|\mathbf{x}-\mathbf{P}|}\chi_{B_R(\mathbf{P})})\chi_2 u_i) \\ &\geq \operatorname{Tr}[\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\mathbf{x}|}\chi_{|\mathbf{x}-\mathbf{P}|<\frac{1}{2}\beta Z^{-t}} - \frac{\nu}{|\mathbf{x}-\mathbf{P}|}\chi_{B_R(\mathbf{P})}]_-,\end{aligned}$$

and by [24, Theorem 2.8] we get

$$\begin{aligned}\sum_{i=1}^{N}(\chi_2 u_i, h\chi_2 u_i) &\geq -CZ^{5/2}\alpha^{1/2} - C\int_{\frac{1}{2}\beta Z^{-t}>|\mathbf{x}-\mathbf{P}|>\alpha}\left(\frac{Z^{5/2}}{|\mathbf{x}|^{5/2}} + \alpha^3\frac{Z^4}{|\mathbf{x}|^4}\right)d\mathbf{x} \\ &\quad -C\int_{R>|\mathbf{x}-\mathbf{P}|>\alpha}\left(\frac{\nu^{5/2}}{|\mathbf{x}-\mathbf{P}|^{5/2}} + \alpha^3\frac{\nu^4}{|\mathbf{x}-\mathbf{P}|^4}\right)d\mathbf{x} \\ &\geq -C\kappa^{1/2}Z^2 - C\beta^{1/2}Z^{5/2-t/2} - C\kappa^2 Z^2. \qquad \text{(B12)}\end{aligned}$$

Here we used that $t < l$ and $Z\alpha = \kappa$.

The outer zone. This region gives the main contribution to the energy. The term in (B10) that we still have to study is

$$\sum_{i=1}^{N}(\chi_3 u_i, h\chi_3 u_i) - D(\rho) \qquad \text{(B13)}$$

We start by estimating the first term in (B13) using coherent states.

We consider again the function $g \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ introduced at the beginning of the proof and we define the function

$$g_s(\mathbf{x}) := (\beta/(8Z^s))^{-\frac{3}{2}}g(8Z^s\mathbf{x}/\beta) = \Phi_s^{\frac{1}{2}}(\mathbf{x}), \qquad \text{(B14)}$$

with s the same parameter as before. For simplicity of notation we write $\tilde{V} := Z/|\mathbf{x}| - \rho * 1/|\mathbf{x}|$. Then

$$\frac{Z}{|\mathbf{x}|} - \rho * \Phi_s * \frac{1}{|\mathbf{x}|} = \tilde{V} * \Phi_s - Z\Phi_s * \frac{1}{|\mathbf{x}|} + \frac{Z}{|\mathbf{x}|}.$$

Since $\mathrm{supp}(g_s) \cap \mathrm{supp}(\chi_3) = \emptyset$ by Newton's Theorem we find

$$\sum_{i=1}^{N} (\chi_3 u_i, h\chi_3 u_i) = \sum_{i=1}^{N} (\chi_3 u_i, (\alpha^{-1}T(\mathbf{p}) - \tilde{V} * \Phi_s)\chi_3 u_i). \tag{B15}$$

We consider the coherent states $g_s^{\mathbf{p},\mathbf{q}}$ defined for $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ by

$$g_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) = g_s(\mathbf{x} - \mathbf{q})e^{-i\mathbf{p}.\mathbf{x}}.$$

The following formulas hold for $f \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C})$

$$\begin{aligned} (f, f) &= \tfrac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q}\, (f, g_s^{\mathbf{p},\mathbf{q}})\, (g_s^{\mathbf{p},\mathbf{q}}, f), \\ (f, V * g_s^2 f) &= \tfrac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q}\, V(\mathbf{q})\, (f, g_s^{\mathbf{p},\mathbf{q}})\, (g_s^{\mathbf{p},\mathbf{q}}, f) \end{aligned} \tag{B16}$$

and

$$\begin{aligned} (f, T(\mathbf{p})f) &= \tfrac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q}\, T(\mathbf{p})\, (f, g_s^{\mathbf{p},\mathbf{q}})\, (g_s^{\mathbf{p},\mathbf{q}}, f) \\ &\quad - \int_{\mathbb{R}^3} d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{q} \overline{f(\mathbf{x})} (L_q f)(\mathbf{x}), \end{aligned} \tag{B17}$$

where L_q has integral kernel

$$L_q(\mathbf{x}, \mathbf{y}) = \frac{\alpha^{-2}}{4\pi^2} |g_s(\mathbf{x} - \mathbf{q}) - g_s(\mathbf{y} - \mathbf{q})|^2 \frac{K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|)}{|\mathbf{x} - \mathbf{y}|^2}.$$

Using these formulas we can rewrite (B15) as follows

$$\begin{aligned} &\sum_{i=1}^{N} (\chi_3 u_i, (\alpha^{-1}T(\mathbf{p}) - \tilde{V} * \Phi_s)\chi_3 u_i) \\ = \; &\tfrac{1}{(2\pi)^3} \alpha^{-1} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q} (T(\mathbf{p}) - \alpha\tilde{V}(\mathbf{q})) \sum_{j=1}^{q} \sum_{i=1}^{N} |(\chi_3 u_i^j, g_s^{\mathbf{p},\mathbf{q}})|^2 \\ &- \alpha^{-1} \sum_{i=1}^{N} \int_{\mathbb{R}^3} d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{q}\, \overline{\chi_3 u_i(\mathbf{x})} (L_{\mathbf{q}} \chi_3 u_i)(\mathbf{x}), \end{aligned} \tag{B18}$$

Here u_i^j is the j-th spin component of u_i. We start by estimating the error term, the last term on the right hand side of (B18). From the definition of $L_{\mathbf{q}}$ it follows

$$L_q(\mathbf{x}, \mathbf{y}) \le \frac{\alpha^{-2}}{4\pi^2} \|\nabla g_s\|_\infty^2 K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|)(\chi_{\mathrm{supp}(g_s)}(\mathbf{x} - \mathbf{q}) + \chi_{\mathrm{supp}(g_s)}(\mathbf{y} - \mathbf{q})),$$

and by the definition of the function g_s

$$\int_{\mathbb{R}^3} L_q(\mathbf{x}, \mathbf{y})\, d\mathbf{q} \le C\|\nabla g\|_\infty^2 \alpha^{-2} \beta^{-2} Z^{2s} K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|).$$

By the estimate above, Schwarz's inequality, (B9) and the choice of s we find

$$\alpha^{-1}\sum_{i=1}^{N}\int_{\mathbb{R}^3}d\mathbf{x}\int_{\mathbb{R}^3}d\mathbf{q}\;\overline{\chi_3 u_i(\mathbf{x})}(L_{\mathbf{q}}\chi_3 u_i)(\mathbf{x})\leq C\|\nabla g\|_\infty^2\beta^{-2}Z^{3/2-t/2}N. \quad \text{(B19)}$$

It remains to study the first term on the right hand side of (B18). In order to get an estimate from below we consider only the negative part of the integrand. Moreover, since if $|\mathbf{q}|<\beta Z^{-t}/8$ then $\operatorname{supp}(\chi_3 g_s^{\mathbf{p},\mathbf{q}})=\emptyset$ (because $Z^{-t}>Z^{-s}$ since $s>t$) we find

$$\begin{aligned}
&\tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3}d\mathbf{p}\int_{\mathbb{R}^3}d\mathbf{q}\;(T(\mathbf{p})-\alpha\tilde V(\mathbf{q}))\sum_{j=1}^{q}\sum_{i=1}^{N}|(\chi_3 u_i^j, g_s^{\mathbf{p},\mathbf{q}})|^2\\
\geq\;&\tfrac{q}{(2\pi)^3}\alpha^{-1}\int_{|\mathbf{q}|\geq\frac18\beta Z^{-t}}d\mathbf{q}\int_{T(\mathbf{p})-\alpha\tilde V(\mathbf{q})\leq 0}d\mathbf{p}\;(T(\mathbf{p})-\alpha\tilde V(\mathbf{q}))=\ldots, \quad \text{(B20)}
\end{aligned}$$

where we also use that $\sum_{i=1}^N|(\chi_3 u_i^j, g_s^{\mathrm{P},\mathrm{Q}})|^2\leq 1$ (Bessel's inequality). We split now the integral as a sum of two terms

$$\begin{aligned}
\ldots\;=\;&\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac12|\mathbf{p}|^2-\tilde V(\mathbf{q})\leq 0\\ |\mathbf{q}|\geq\frac18\beta Z^{-t}}}d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\tilde V(\mathbf{q}))\\
+\;&\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\geq\alpha\tilde V(\mathbf{q})\geq T(\mathbf{p})\\ |\mathbf{q}|\geq\frac18\beta Z^{-t}}}d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\tilde V(\mathbf{q})). \quad \text{(B21)}
\end{aligned}$$

We consider these two terms separately. The second term in (B21) gives a lower order contribution. Indeed

$$\begin{aligned}
&\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\geq\alpha\tilde V(\mathbf{q})\geq T(\mathbf{p})\\ |\mathbf{q}|\geq\frac18\beta Z^{-t}}}d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\tilde V(\mathbf{q}))\\
\geq\;&-\tfrac{q}{(2\pi)^3}\iint_{\substack{(\alpha^2[\tilde V(\mathbf{q})]_+^2+2[\tilde V(\mathbf{q})]_+)^{\frac12}\geq|\mathbf{p}|\geq(2[\tilde V(\mathbf{q})]_+)^{\frac12}\\ |\mathbf{q}|\geq\frac18\beta Z^{-t}}}d\mathbf{q}d\mathbf{p}\;[\tilde V(\mathbf{q})]_+=\ldots,
\end{aligned}$$

and computing the $\mathbf{p}$-integral

$$\cdots=-C\int_{|\mathbf{q}|\geq\frac18\beta Z^{-t}}d\mathbf{q}\;[\tilde V(\mathbf{q})]_+^{\frac52}((1+\frac{\alpha^2}{2}[\tilde V(\mathbf{q})]_+)^{\frac32}-1)=\ldots.$$

Using $(1+x)^{\frac32}\leq 1+\frac32 x+\frac38 x^2$ and that $[\tilde V(\mathbf{q})]_+\leq Z/|\mathbf{q}|$ we get computing the integral

$$\begin{aligned}
\ldots\;=\;&-C\alpha^2\textstyle\int_{|\mathbf{q}|\geq\frac18\beta Z^{-t}}d\mathbf{q}\;[\tilde V(\mathbf{q})]_+^{\frac72}(1+\frac{\alpha^2}{8}[\tilde V(\mathbf{q})]_+)\\
\geq\;&-C\beta^{-\frac12}\kappa^2 Z^{3/2+t/2}-C\kappa^4\beta^{-\frac32}Z^{1/2+3t/2}.
\end{aligned} \quad \text{(B22)}$$

Here we use that $Z\alpha = \kappa$.
Since $\sqrt{1+x} \geq 1 + x/2 - x^3/8$ for all $x > 0$, we have

$$T(\mathbf{p}) \geq \alpha \tfrac{1}{2}|\mathbf{p}|^2 - \alpha^3 \tfrac{1}{8}|\mathbf{p}|^4,$$

and, for the first term on the right hand side of (B21), we obtain

$$\begin{aligned} &\tfrac{q}{(2\pi)^3}\alpha^{-1} \iint_{\substack{\frac{1}{2}|\mathbf{p}|^2 - \tilde{V}(\mathbf{q}) \leq 0 \\ |\mathbf{q}| \geq \frac{1}{8}\beta Z^{-t}}} d\mathbf{q} d\mathbf{p}\, (T(\mathbf{p}) - \alpha \tilde{V}(\mathbf{q})) \geq \\ \geq\ &\tfrac{q}{(2\pi)^3} \iint_{\substack{\frac{1}{2}|\mathbf{p}|^2 - \tilde{V}(\mathbf{q}) \leq 0 \\ |\mathbf{q}| \geq \frac{1}{8}\beta Z^{-t}}} d\mathbf{q} d\mathbf{p}\, (\tfrac{1}{2}|\mathbf{p}|^2 - \tfrac{1}{8}\alpha^2|\mathbf{p}|^4 - \tilde{V}(\mathbf{q})) = \ldots. \end{aligned}$$

Computing now the integral with respect to $\mathbf{p}$, we find

$$\cdots = -\tfrac{2^{\frac{3}{2}} q}{15\pi^2} \int_{|\mathbf{q}| > \frac{1}{8}\beta Z^{-t}} [\tilde{V}(\mathbf{q})]_+^{\frac{5}{2}}\, d\mathbf{q} - C\alpha^2 \int_{|\mathbf{q}| > \frac{1}{8}\beta Z^{-t}} [\tilde{V}(\mathbf{q})]_+^{\frac{7}{2}}\, d\mathbf{q}. \tag{B23}$$

We see that the second term on the right hand side of (B23) gives a lower order contribution since it is of the same order as the one in (B22).
Collecting together (B10), (B11), (B12), (B15), (B18), (B19), (B22) and (B23)

$$\langle \psi, H_{\mathbf{P}} \psi \rangle \quad \geq \quad -C(\beta^{\frac{1}{2}} + \beta^{-2}) Z^{5/2 - t/2} - \tfrac{2^{\frac{3}{2}} q}{15\pi^2} \int_{\mathbb{R}^3} [\tilde{V}(\mathbf{q})]_+^{\frac{5}{2}}\, d\mathbf{q} - D(\rho)\,. \tag{B24}$$

Here we used also that $N < 2Z + 1$, the choice of s and that $t \leq 3/5$.
Now we choose $\rho = \rho^{\mathrm{TF}}$ the minimizer of the TF-energy functional of a neutral atom with Coulomb potential and nuclear charge Z. Hence ρ^{TF} satisfies the TF-equation

$$\tfrac{1}{2}\big(\tfrac{6\pi^2}{q}\big)^{\frac{2}{3}} \rho^{\mathrm{TF}}(\mathbf{x})^{\frac{2}{3}} = [\tilde{V}(\mathbf{x})]_+,$$

since $\tilde{V}$ is the TF-mean field potential. Notice that here we use that the chemical potential of a neutral atom is zero. By the choice of ρ from the TF-equation it follows from (B24) that

$$\begin{aligned} \langle \psi, H_{\mathbf{P}} \psi \rangle \quad &\geq \quad -C(\beta^{\frac{1}{2}} + \beta^{-2}) Z^{5/2 - t/2} + \tfrac{3}{10}\big(\tfrac{6\pi^2}{q}\big)^{\frac{2}{3}} \int_{\mathbb{R}^3} d\mathbf{x}\, \rho^{\mathrm{TF}}(\mathbf{x})^{\frac{5}{3}} \\ &\qquad -Z \int_{\mathbb{R}^3} \frac{\rho^{\mathrm{TF}}(\mathbf{x})}{|\mathbf{x}|}\, d\mathbf{x} + D(\rho^{\mathrm{TF}}) \\ &= \quad \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - C(\beta^{\frac{1}{2}} + \beta^{-2}) Z^{5/2 - t/2}\,. \end{aligned}$$

The claim follows. □

Proposition B.2. *Let ρ^{TF} be the minimizer of the TF-energy functional of a neutral atom with nuclear charge Z. Let $Z\alpha = \kappa$ be fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$.*

Then there is a constant depending only on κ and q such that for all $\{u_i\}_{i=1}^N \subset H^{\frac{1}{2}}(\mathbb{R}^3;\mathbb{C}^q)$ orthonormal in $L^2(\mathbb{R}^3)$ we have

$$\sum_{i=1}^N (u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})u_i) - D(\rho^{\mathrm{TF}}) \geq \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - CZ^{2+\frac{1}{5}}\,,$$

with $D(\cdot) = D(\cdot,\cdot)$ the Coulomb scalar product.

Proof. Since $\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = -e_0 Z^{\frac{7}{3}}$ (see (12)) to prove the claim it is sufficient to show that the TF-energy gives a lower bound to the quantum energy modulo lower order terms. In the proof we localize the energy separating the contribution from the region near the nucleus to the one far away. The region far away from the nuclei will give the TF-energy.
In the proof C denotes a generic universal positive constant.
Choice of the localization. The localization will be given by the functions $\chi_1 \in C_0^\infty(\mathbb{R}^3)$ and $\chi_2 \in C^\infty(\mathbb{R}^3)$ such that: $0 \leq \chi_1, \chi_2 \leq 1$, $\chi_1^2 + \chi_2^2 = 1$ in $\mathbb{R}^3$,

$$\chi_1(\mathbf{x}) := \begin{cases} 1 & \text{if } |\mathbf{x}| < 2Z^{-3/5}, \\ 0 & \text{if } |\mathbf{x}| > 3Z^{-3/5}. \end{cases} \tag{B25}$$

Moreover we ask that

$$\|\nabla\chi_1\|_\infty, \|\nabla\chi_2\|_\infty \leq 2^2 Z^{3/5}. \tag{B26}$$

The localization in the energy expectation. We insert now the localization in the energy expectation. From Theorem 2.1 we find

$$\begin{aligned} &\sum_{i=1}^N (u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})u_i) - D(\rho^{\mathrm{TF}}) \qquad \text{(B27)} \\ \geq\ &\sum_{i=1}^N \sum_{j=1}^2 (\chi_j u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})\chi_j u_i) - D(\rho^{\mathrm{TF}}) - \alpha^{-1}\sum_{i=1}^N\sum_{j=1}^2 (u_i, L_j u_i), \end{aligned}$$

with L_j is the operator (defined in Theorem 2.1) that gives the error due to the localization in the kinetic energy. We first estimate this error term. Since $N \leq 2Z+1$ we find as in (B8) that

$$\alpha^{-1}\sum_{i=1}^N\sum_{j=1}^2 (u_i, L_j u_i) \leq CZ^{6/5}N \leq CZ^{2+1/5}\,. \tag{B28}$$

Near the nucleus. Since

$$\sum_{i=1}^N (\chi_1 u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})\chi_1 u_i) \geq \mathrm{Tr}[\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}}\chi_{|\mathbf{x}|<3Z^{-3/5}}]_-,$$

by Theorem 2.10 with $R = 3Z^{-3/5}$ we find

$$\sum_{i=1}^{N}(\chi_1 u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})\chi_1 u_i) \geq -CZ^{2+1/5} - C\kappa^2 Z^2. \tag{B29}$$

Here we use that $Z\alpha = \kappa$.

The outer zone. This region gives the main contribution to the energy.

Let $g \in C_0^\infty(\mathbb{R}^3)$, $g \geq 0$ be spherically symmetric with $\mathrm{supp}(g) \subset B_1(0)$ and such that $\|g\|_2 = 1$. Starting from these g we define $\Phi_Z(\mathbf{x}) := (Z^{-3/5})^{-3} g^2(\mathbf{x}Z^{3/5})$ and

$$g_Z(\mathbf{x}) := (Z^{-3/5})^{-\frac{3}{2}} g(\mathbf{x}Z^{3/5}) = \Phi_Z^{\frac{1}{2}}(\mathbf{x}).$$

Since $\mathrm{supp}(g_Z) \cap \mathrm{supp}(\chi_2) = \emptyset$ by Newton's Theorem we find

$$\sum_{i=1}^{N}(\chi_2 u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})\chi_2 u_i) = \sum_{i=1}^{N}(\chi_2 u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}} * \Phi_Z)\chi_2 u_i). \tag{B30}$$

We consider the coherent states $g_Z^{\mathbf{p},\mathbf{q}}$ defined for $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ by

$$g_Z^{\mathbf{p},\mathbf{q}}(\mathbf{x}) = g_Z(\mathbf{x} - \mathbf{q})e^{-i\mathbf{p}.\mathbf{x}}.$$

Using formulas (B16) and (B17) we can rewrite (B30) as follows

$$\begin{aligned}
&\sum_{i=1}^{N}(\chi_2 u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}} * g_Z^2)\chi_2 u_i) \\
= \;& \tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3} d\mathbf{p}\int_{\mathbb{R}^3} d\mathbf{q}(T(\mathbf{p}) - \alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\sum_{j=1}^{q}\sum_{i=1}^{N}|(\chi_2 u_i^j, g_Z^{\mathbf{p},\mathbf{q}})|^2 \\
& - \alpha^{-1}\sum_{i=1}^{N}\int_{\mathbb{R}^3} d\mathbf{x}\int_{\mathbb{R}^3} d\mathbf{q}\; \overline{\chi_2 u_i(\mathbf{x})}(L_{\mathbf{q}}\chi_2 u_i)(\mathbf{x}),
\end{aligned} \tag{B31}$$

Here u_i^j is the j-th spin component of u_i. We start by estimating the error term, the last term on the right hand side of (B31). We find as in (B19) that

$$\alpha^{-1}\sum_{i=1}^{N}\int_{\mathbb{R}^3} d\mathbf{x}\int_{\mathbb{R}^3} d\mathbf{q}\; \overline{\chi_2 u_i(\mathbf{x})}(L_{\mathbf{q}}\chi_2 u_i)(\mathbf{x}) \leq C\|\nabla g\|_\infty^2 Z^{6/5}N. \tag{B32}$$

It remains to study the first term on the right hand side of (B31). In order to get an estimate from below we consider only the negative part of the integrand. Moreover, since if $|\mathbf{q}| < Z^{-3/5}$ then $\mathrm{supp}(\chi_2 g_Z^{\mathbf{p},\mathbf{q}}) = \emptyset$ we find

$$\begin{aligned}
&\tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3} d\mathbf{p}\int_{\mathbb{R}^3} d\mathbf{q}\;(T(\mathbf{p}) - \alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\sum_{j=1}^{q}\sum_{i=1}^{N}|(\chi_2 u_i^j, g_Z^{\mathbf{p},\mathbf{q}})|^2 \\
\geq\; & \tfrac{q}{(2\pi)^3}\alpha^{-1}\int_{|\mathbf{q}|\geq Z^{-3/5}} d\mathbf{q}\int_{T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})\leq 0} d\mathbf{p}\;(T(\mathbf{p}) - \alpha\varphi^{\mathrm{TF}}(\mathbf{q})) = \ldots,
\end{aligned} \tag{B33}$$

where we also use that $\sum_{i=1}^N |(\chi_3 u_i^j, g_Z^{\mathrm{P,Q}})|^2 \le 1$ (Bessel's inequality). We split now the integral as a sum of two terms

$$\begin{aligned} \cdots &= \tfrac{q}{(2\pi)^3}\alpha^{-1} \iint_{\substack{\frac12|\mathbf{p}|^2-\varphi^{\mathrm{TF}}(\mathbf{q})\le 0\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})) \\ &+ \tfrac{q}{(2\pi)^3}\alpha^{-1} \iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\ge\alpha\varphi^{\mathrm{TF}}(\mathbf{q})\ge T(\mathbf{p})\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})). \quad \text{(B34)}\end{aligned}$$

We consider these two terms separately. The second term in (B34) gives a lower order contribution. Indeed

$$\begin{aligned} &\tfrac{q}{(2\pi)^3}\alpha^{-1} \iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\ge\alpha\varphi^{\mathrm{TF}}(\mathbf{q})\ge T(\mathbf{p})\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})) \\ \ge\; & -\tfrac{q}{(2\pi)^3} \iint_{\substack{(\alpha^2[\varphi^{\mathrm{TF}}]_+^2+2[\varphi^{\mathrm{TF}}]_+)^{\frac12}\ge|\mathbf{p}|\ge(2[\varphi^{\mathrm{TF}}(\mathbf{q})]_+)^{\frac12}\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;[\varphi^{\mathrm{TF}}(\mathbf{q})]_+ = \ldots,\end{aligned}$$

and computing the integral in $\mathbf{p}$

$$\cdots = -C\int_{|\mathbf{q}|\ge Z^{-3/5}} d\mathbf{q}\;[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac52}((1+\frac{\alpha^2}{2}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+)^{\frac32}-1) = \ldots.$$

Using $(1+x)^{\frac32}\le 1+\frac32 x+\frac38 x^2$ and that $[\varphi^{\mathrm{TF}}(\mathbf{q})]_+ \le Z/|\mathbf{q}|$ we get computing the integral

$$\begin{aligned} \cdots &= -C\alpha^2\int_{|\mathbf{q}|\ge Z^{-3/5}} d\mathbf{q}\;[\varphi^{\mathrm{TF}}]_+^{\frac72}(1+\frac{\alpha^2}{8}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+) \\ &\ge -C\kappa^2 Z^{2-\frac15} - C\kappa^4 Z^{\frac75}. \end{aligned} \quad \text{(B35)}$$

Since $\sqrt{1+x}\ge 1+x/2-x^3/8$ for all $x\ge 0$, we have

$$T(\mathbf{p}) \ge \alpha\tfrac12|\mathbf{p}|^2 - \alpha^3\tfrac18|\mathbf{p}|^4,$$

and, for the first term on the right hand side of (B34), we obtain

$$\begin{aligned} &\tfrac{q}{(2\pi)^3}\alpha^{-1} \iint_{\substack{\frac12|\mathbf{p}|^2-\varphi^{\mathrm{TF}}(\mathbf{q})\le 0\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})) \ge \\ \ge\; & \tfrac{q}{(2\pi)^3} \iint_{\substack{\frac12|\mathbf{p}|^2-\varphi^{\mathrm{TF}}(\mathbf{q})\le 0\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(\tfrac12|\mathbf{p}|^2-\tfrac18\alpha^2|\mathbf{p}|^4-\varphi^{\mathrm{TF}}(\mathbf{q})) = \ldots.\end{aligned}$$

Computing now the integral with respect to $\mathbf{p}$, we find

$$\cdots = -\tfrac{2^{\frac32}q}{15\pi^2}\int_{|\mathbf{q}|>Z^{-3/5}}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac52}\,d\mathbf{q} - C\alpha^2\int_{|\mathbf{q}|>Z^{-3/5}}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac72}\,d\mathbf{q}. \quad \text{(B36)}$$

We see that the second term on the right hand side of (B36) gives a lower order contribution since it is of the same order as the one in (B35).
Starting from (B27), by (B28), (B29), (B32), (B35) and (B36) we find

$$\sum_{i=1}^{N}(u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})u_i)-D(\rho^{\mathrm{TF}}) \tag{B37}$$
$$\geq\ -C(Z^{2+1/5}+Z^2+Z^{2-1/5}+Z^{7/5})-\frac{2^{\frac{3}{2}}q}{15\pi^2}\int_{\mathbb{R}^3}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q}-D(\rho^{\mathrm{TF}}).$$

The result follows from the TF-equation. □

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On the Solutions of Quadratic Diophantine Equations

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Abstract. We determine a finite set of representatives of the set of local solutions in a maximal lattice modulo the stabilizer of the lattice in question for a quadratic Diophantine equation. Our study is based on the works of Shimura on quadratic forms, especially [AQC] and [IQD]. Indeed, as an application of the result, we present a criterion (in both global and local cases) of the maximality of the lattice of (11.6a) in [AQC]. This gives an answer to the question (11.6a). As one more global application, we investigate primitive solutions contained in a maximal lattice for the sums of squares on each vector space of dimension 4, 6, 8, or 10 over the field of rational numbers.

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1 Introduction

In this paper we study quadratic forms over global and local fields of characteristic zero, i.e. over number fields and their p-adic completions. Let F be a field of one of these two types. We let $\mathfrak{g}$ denote the ring of all integers in F (in both global and local cases). We denote by $\mathfrak{p}$ the maximal ideal of $\mathfrak{g}$ in the local case. Throughout the paper we mainly follow the notion and the notation in Shimura's book [AQC] and the paper [IQD]. We denote by V an n-dimensional vector space over F. Let $\varphi : V \times V \to F$ be a nondegenerate symmetric F-bilinear form. We denote by $\varphi[x]$ the quadratic form $\varphi(x, x)$ on V. By a maximal lattice L in V with respect to φ, we understand a $\mathfrak{g}$-lattice L in V, which is maximal among $\mathfrak{g}$-lattices on which the values $\varphi[x]$ are contained in $\mathfrak{g}$. For simplicity, when φ is fixed on V, we will often refer to a maximal lattice in V, omitting reference to the φ needed to define it. All results in the paper concern only maximal lattices in V. Let SO^φ be the special orthogonal group of φ. In this paper we consider the set of the solutions of the quadratic Diophantine equation $\varphi[x] = q$ in L, that is

$$L[q] = \{x \in L \mid \varphi[x] = q\},$$

and

$$L[q, \mathfrak{b}] = \{x \in V \mid \varphi[x] = q, \varphi(x, L) = \mathfrak{b}\},$$

where $q \in \mathfrak{g} \cap F^\times$ and a fractional ideal $\mathfrak{b}$ of F.

Assume now that F is local, put $C(L) = \{\gamma \in SO^\varphi \mid L\gamma = L\}$, and take $h \in L$ such that $\varphi[h] \neq 0$. It was shown by Shimura that there exists a finite subset A of SO^φ such that

$$L[\varphi[h]] = \bigsqcup_{\alpha \in A} h\alpha C(L)$$

([AQC, Theorem 10.3]) and

$$\#\{L[q, \mathfrak{b}]/C(L)\} \leq 1 \text{ if } n > 2$$

([IQD, Theorem 1.3]). Note that [AQC, Theorem 10.3] is true even when L is not maximal. In Theorem 3.5 we shall obtain, using the proof of [AQC, Theorem 10.3], an explicit complete set $\{h\alpha\}_{\alpha \in A}$ of representatives for $L[\varphi[h]]/C(L)$. Also, we show that

$$L[\varphi[h]] = \begin{cases} L[\varphi[h], 2^{-1}\mathfrak{p}^{\tau(\varphi[h])}] & \text{if } \varphi \text{ is anisotropic,} \\ \bigsqcup_{i=0}^{\tau(\varphi[h])} L[\varphi[h], 2^{-1}\mathfrak{p}^i] & \text{if } \varphi \text{ is isotropic,} \end{cases}$$

with the value $\tau(\varphi[h])$; see Theorem 3.5.

As a result of this theorem we prove Theorem 5.3: Suppose F is local and $n \geq 2$. Then

$$L \cap (Fh)^\perp \text{ is maximal in } (Fh)^\perp \text{ if and only if } h \in L[\varphi[h], 2^{-1}\mathfrak{p}^{\tau(\varphi[h])}]$$

for $h \in L$ such that $\varphi[h] \neq 0$. Here $(Fh)^\perp = \{x \in V \mid \varphi(x, h) = 0\}$. We also obtain the global version of the maximality of the lattice $L \cap (Fh)^\perp$ in $(Fh)^\perp$ in Theorem 6.3. This theorem answers the question raised in [AQC, (11.6a)]. As a global application of Theorem 3.5, in Theorem 7.5 we give the criterion of the existence of solutions contained in $L[q, \mathbf{Z}]$ and $L[q, 2^{-1}\mathbf{Z}]$ in both cases when q is a squarefree positive integer, by taking $V = \mathbf{Q}_n^1$ ($4 \leq n \leq 10$, n even), the sums of squares as φ, and a maximal lattice L in V. It is known that $L[q] = L[q, 2^{-1}\mathbf{Z}] \sqcup L[q, \mathbf{Z}]$; see [AQC, (12.17)]. For example, when $n = 6$, the set $L[q, \mathbf{Z}] = \emptyset$ if and only if $q - 1 \in 4\mathbf{Z}$. When $n = 10$, the genus of L consists of two SO^φ-classes $L_{10}SO^\varphi$ and ΛSO^φ (cf. [CGQ, §3.2]). In this case,

$$L[q, \mathbf{Z}] = \emptyset \text{ if and only if } \begin{cases} L \in L_{10}SO^\varphi, q = 1 \text{ or } q - 3 \in 4\mathbf{Z}; \text{ or} \\ L \in \Lambda SO^\varphi, q - 3 \in 4\mathbf{Z}. \end{cases}$$

We summarize the contents of the paper. In Section 2 we recall the notion of Shimura [AQC] and [IQD] and introduce the basic facts of a local Witt decomposition with respect to φ. In Sections 3 through 5 we treat local cases. In Section 3 we introduce the result obtained from the proof of [AQC, Theorem 10.3] and state the first result. In Section 4 we prove Theorem 3.5. In Section 5 we shall give a criterion of the maximality of the lattice $L \cap (Fh)^{\perp}$ in $(Fh)^{\perp}$ in the local case. In Section 6 we prove the global version of Theorem 5.3. In Section 7 we prove Theorem 7.5.

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Notations and Conventions As usual, $\mathbf{Z}$ (resp. $\mathbf{Z}_p$) is the ring of rational (resp. p-adic) integers, $\mathbf{Q}$ (resp. $\mathbf{Q}_p$) the field of rational (resp. p-adic) numbers. In this paper we consider the base field F in two cases. One is a global field and the other is a local field. When we do not need to specify the case of F, we call it only "a field".

If R is an associative ring with identity element, then $R^{\times}$ is the group of units of R. If K is a finite algebraic extension of a field F, then $D_{K/F}$ denotes the relative discriminant of K over F. Let $\mathfrak{d}_{K/F}$ be the different of K relative to F.

If F is a local field, then for $x \in F^{\times}$, put

$$\xi(x) = \begin{cases} 1 & \text{if } \sqrt{x} \in F, \\ -1 & \text{if } F(\sqrt{x}) \text{ is an unramified quadratic extension of } F, \\ 0 & \text{if } F(\sqrt{x}) \text{ is a ramified quadratic extension of } F \end{cases}$$

as in [NRQ, (3.3.1)].

If F is the field of quotients of a Dedekind domain $\mathfrak{g}$ and V an n-dimensional vector space over F, then by a $\mathfrak{g}$-lattice in V, we understand a finitely generated $\mathfrak{g}$-module in V that spans V over F. In particular, if $\mathfrak{a}$ is a $\mathfrak{g}$-lattice in F, we call $\mathfrak{a}$ a $\mathfrak{g}$-ideal of F. We write $\dim_F(V)$ for the dimension of V over F. We let $GL(V, F)$ denote the group of all F-linear automorphisms of V. If $R = F$ or $\mathfrak{g}$, then we write R_n^m for the ring of all $m \times n$-matrices with entries in R and let $GL_n(R) = (R_n^n)^{\times}$.

If X is a set, then $\#X$ denotes the cardinality of X. If X is a disjoint union of its subsets $Y_1, \cdots, Y_m$, we write $X = \bigsqcup_{i=1}^m Y_i$ or $X = Y_1 \sqcup \cdots \sqcup Y_m$. For a subgroup H of a group G, we let $[G : H] = \#(H \setminus G)$.

We denote by δ_{ij} Kronecker's delta. For a real number a, we let $[a]$ denote the greatest integer not greater than a.

2 Preliminaries

2.1. Let F be a field and we consider the pair (V, φ) as in the introduction. Define

$$SO^{\varphi}(V) = \{\alpha \in GL(V, F) \mid \det(\alpha) = 1,\ \varphi[x\alpha] = \varphi[x] \text{ for all } x \in V\}.$$

We understand that $GL(V, F)$ acts on V on the right. Let $\varphi_0 = [\varphi(x_i, x_j)]_{i,j=1}^n$ for an F-basis $\{x_i\}_{i=1}^n$ of V, then $\varphi_0 \in GL_n(F)$ such that $\varphi_0 = {}^t\varphi_0$. Define the discriminant of (V, φ) by

$$\delta(\varphi) = \delta(V, \varphi) = (-1)^{n(n-1)/2} \det(\varphi_0) F^{\times 2}. \tag{2.1}$$

Let $A(V) = A(V, \varphi)$ be the Clifford algebra of φ (cf. [AQC, Chap. I Section 2]). We say that (V_1, φ_1) is isomorphic to (V_2, φ_2) if there is an F-linear isomorphism f of V_1 onto V_2 such that $\varphi_1[x] = \varphi_2[xf]$ for any $x \in V_1$. If W is a subspace of V, then we always consider (W, ψ), where ψ is the restriction of φ to W ($\psi[x] = \varphi[x]$ for $x \in W$).
For a $\mathfrak{g}$-lattice Λ in V, put

$$\tilde{\Lambda} = \Lambda^{\sim} = \{x \in V \mid \varphi(x, \Lambda) \subset 2^{-1}\mathfrak{g}\}, \tag{2.2}$$

$$C(\Lambda) = \{\gamma \in SO^{\varphi}(V) \mid \Lambda\gamma = \Lambda\}. \tag{2.3}$$

By an integral lattice L in V (with respect to φ), we understand a $\mathfrak{g}$-lattice L in V such that $\varphi[x] \in \mathfrak{g}$ for every $x \in L$. We call L maximal (with respect to φ) if it is maximal among integral lattices in V. We note that $L \subset \tilde{L}$ when L is an integral lattice in V.

2.2. Here we assume that F is a local field and L is a maximal lattice in V with respect to φ. Considering the maximality of L, we have a Witt decomposition by [AQC, Lemma 6.5];

$$V = Z + \sum_{i=1}^{r} (Ff_i + Fe_i), \quad L = N + \sum_{i=1}^{r} (\mathfrak{g}f_i + \mathfrak{g}e_i), \tag{2.4}$$

where

$$\varphi(e_i, e_j) = \varphi(f_i, f_j) = 0, \quad \varphi(e_i, f_j) = 2^{-1}\delta_{ij}, \tag{2.5}$$

$$Z = \{z \in V \mid \varphi(e_i, z) = \varphi(f_i, z) = 0 \text{ for all } i\}, \tag{2.6}$$

$$N = \{z \in Z \mid \varphi[z] \in \mathfrak{g}\}. \tag{2.7}$$

Here the restriction of φ to Z is anisotropic and N is a unique maximal lattice in Z by [AQC, Lemma 6.4]. We say that Z is a core subspace of V with respect to φ. Until the end of Section 5, we fix these decompositions. Put $t = \dim_F(Z)$ then $n = 2r + t$. We have $t \leq 4$ by [AQC, Theorem 7.6(ii)]. We call t the core dimension of (V, φ).

2.3. We introduce here the basic notions of (Z,φ) and of N, which play an important role in this paper. Note that we use the same letters c and δ, for simplification, in the following different cases (I) (2.10), (II) (2.13), and (III) (2.15).
(I) Assume $t=1$ (cf. [AQC, §7.1 and §7.7(I)] and [IQD, §1.5(A)]). Take $g \in Z$ such that

$$N = \mathfrak{g}g \tag{2.8}$$

and put

$$c = \varphi[g]. \tag{2.9}$$

Then $Z = Fg$ and $\varphi[xg] = cx^2$ for $x \in F$. Furthermore we obtain $c \in \mathfrak{g}^\times$ (resp. $c\mathfrak{g} = \mathfrak{p}$) if $\delta(\varphi) \cap \mathfrak{g} \neq \emptyset$ (resp. $\delta(\varphi) \cap \mathfrak{g} = \emptyset$) by (2.7). Put

$$c\mathfrak{g} = \mathfrak{p}^\delta \text{ with } \delta \in \mathbf{Z}. \tag{2.10}$$

By (2.2) and (2.8), we easily see that

$$\tilde{N} = 2^{-1}\mathfrak{p}^{-\delta}g. \tag{2.11}$$

(II) Next suppose $t=2$ (cf. [AQC, §7.2 and §7.7(II)]). We can take $g_1, g_2 \in Z$ such that $Z = Fg_1 + Fg_2$ and $\varphi(g_1, g_2) = 0$ by [EPE, Lemma 1.8]. Put

$$b = \varphi[g_1] \text{ and } c = \varphi[g_2]. \tag{2.12}$$

Put $K = F + Fg_1g_2$ in $A(Z)$. Then K is a quadratic extension of F, which is isomorphic to $F(\sqrt{-bc})$, $Z = Kg_2$, and $\varphi[xg_2] = cN_{K/F}(x)$ for $x \in K$. We may assume $c \in \mathfrak{g}^\times$ or $c\mathfrak{g} = \mathfrak{p}$. Moreover when K is a ramified extension of F, we can take $c \in \mathfrak{g}^\times$. Then by (2.7) we have $N = \mathfrak{r}g_2$ if K is either unramified or ramified, where $\mathfrak{r}$ is the valuation ring of K. We put

$$c\mathfrak{g} = \mathfrak{p}^\delta \text{ with } \delta \in \mathbf{Z}. \tag{2.13}$$

(III) Suppose $t=3$ (cf. [AQC, §7.3 and §7.7(III)] and [IQD, §1.5(B)]). There exist $g_i \in Z$ such that $Z = Fg_1 + Fg_2 + Fg_3$ and $\varphi(g_i, g_j) = 0$ if $i \neq j$ by [EPE, Lemma 1.8]. Put

$$c = \varphi[g_1]\varphi[g_2]\varphi[g_3]. \tag{2.14}$$

Then we can take $c \in \mathfrak{g}^\times$ (resp. $c\mathfrak{g} = \mathfrak{p}$) if $\delta(\varphi) \cap \mathfrak{g} \neq \emptyset$ (resp. $\delta(\varphi) \cap \mathfrak{g} = \emptyset$). We put

$$c\mathfrak{g} = \mathfrak{p}^\delta \text{ with } \delta \in \mathbf{Z}. \tag{2.15}$$

Put $\zeta = g_1g_2g_3$, $T = Fg_1g_2 + Fg_2g_3 + Fg_3g_1$, and $B = F + T$ in $A(Z)$. Then B is a division quaternion algebra over F and $T = \{x \in B \mid x + x^\iota = 0\}$, where

ι is the main involution of B. Moreover we have $Z = T\zeta$ and $\varphi[x\zeta] = cxx^\iota$ for $x \in T$. Then by (2.7),

$$N = (T \cap \mathfrak{P}^{-\delta})\zeta, \tag{2.16}$$

where $\mathfrak{P} = \{x \in B \mid xx^\iota \in \mathfrak{p}\}$. By [AQC, Theorem 5.13], there exist an unramified quadratic extension K over F and an element $\omega \in B$ such that $B = K + K\omega$, $a\omega = \omega a^\iota$ for each $a \in K$, and $\omega^2 \in \pi\mathfrak{g}^\times$. Here π is a prime element of F. Let $\mathfrak{r}$ be the valuation ring of K. There exists $u \in \mathfrak{r}$ such that $\mathfrak{r} = \mathfrak{g}[u]$ and $u - u^\iota \in \mathfrak{r}^\times$ by [AQC, Lemma 5.7]. Put $v = u - u^\iota$. Then $T = Fv + K\omega$. For $a, \alpha \in \mathfrak{g}$ and $b, \beta \in \mathfrak{r}$,

$$\varphi[(av + b\omega^{1-2\delta})\zeta] = -c(a^2v^2 + \omega^{2(1-2\delta)}N_{K/F}(b)), \tag{2.17}$$

(2.18)
$$\varphi((av + b\omega^{1-2\delta})\zeta, (\alpha v + \beta\omega^{1-2\delta})\zeta) = -2^{-1}c(2a\alpha v^2 + \omega^{2(1-2\delta)}Tr_{K/F}(b\beta^\iota)).$$

From (2.16) and (2.17),

$$N = (\mathfrak{g}v + \mathfrak{r}\omega^{1-2\delta})\zeta = (\mathfrak{g}v + \mathfrak{g}\omega^{1-2\delta} + \mathfrak{g}u\omega^{1-2\delta})\zeta. \tag{2.19}$$

From (2.2) and (2.19),

$$\tilde{N} = (2^{-1}\mathfrak{p}^{-\delta}v + \mathfrak{r}\omega^{-1})\zeta. \tag{2.20}$$

Put $Tr_{B/F}(x) = x + x^\iota$ and $N_{B/F}(x) = xx^\iota$ for $x \in B$.

(IV) Finally assume $t = 4$ (cf. [AQC, Theorem 7.5 and §7.7(IV)]). There exist a division quaternion algebra B over F and an F-linear isomorphism $\gamma : B \to Z$ such that $\varphi[x\gamma] = xx^\iota$ for $x \in B$, where ι is the main involution of B. Then $N = \mathfrak{O}\gamma$. Here $\mathfrak{O}$ is the unique maximal order of B.

3 A complete set of representatives for $L[q]/C(L)$

Until the end of Section 5, we assume that F is a local field and L is a maximal lattice in V with respect to φ. In this section, we first introduce the facts obtained from the proof of [AQC, Theorem 10.3]. After that, we state our first main theorem.

3.1. We suppose that V and L are represented as in (2.4). If $r \geq 1$, put $M = N + \sum_{i=2}^{r}(\mathfrak{g}f_i + \mathfrak{g}e_i)$. We consider $M = N$ if $r = 1$. Then

$$L = \mathfrak{g}f_1 + M + \mathfrak{g}e_1 \tag{3.1}$$

for every $r \geq 1$. For $0 \leq i \in \mathbf{Z}$ and $q \in \mathfrak{g} \cap F^\times$, put

$$X_i(q) = \{x \in M \mid \varphi[x] - q \in \mathfrak{p}^i\}. \tag{3.2}$$

Note that $X_i(q) \supset X_{i+1}(q)$. Hereafter we take a prime element π of F and fix it.

We obtain the following theorem from the proof of [AQC, Theorem 10.3].

3.2 Theorem. (Shimura) *Let the notation be as above. Let $h \in L$ such that $\varphi[h] \neq 0$ and $\nu \in \mathbf{Z}$ such that $\varphi[h]\mathfrak{g} = \mathfrak{p}^\nu$. Put $C = C(L)$ in the notation of (2.3). Let t, e_1, and f_1 be as in §2.2.*
(1) *Suppose $r = 0$. Then*

$$L[\varphi[h]] = \begin{cases} hC \sqcup (-h)C, \quad C = \{1\} & \text{if } t = 1, \\ hC & \text{if } t > 1. \end{cases}$$

(2) *Suppose $n = 2r = 2$. Then $L[\varphi[h]] = \bigsqcup_{i=0}^{\nu} (\pi^i f_1 + \varphi[h]\pi^{-i} e_1)C$.*
(3) *Suppose $n > 2$, $r > 0$, and $M[\varphi[h]] = \emptyset$. Put*

$$\kappa_0 = \min(\{k \in \mathbf{Z} \mid X_k(\varphi[h]) = \emptyset\}). \tag{3.3}$$

Then

$$L[\varphi[h]] = \bigcup_{i=0}^{\kappa_0 - 1} \bigcup_{b \in X_i(\varphi[h])/\mathfrak{p}^i M} [\pi^i f_1 + b + \pi^{-i}(\varphi[h] - \varphi[b])e_1]C.$$

Here b runs over all elements of $X_i(\varphi[h])/\mathfrak{p}^i M$.
(4) *Suppose that $n > 2$, $r > 0$, $M[\varphi[h]] \neq \emptyset$, and that there exists a finite subset B of $M[\varphi[h]]$ such that $M[\varphi[h]] = \sqcup_{b \in B} bC(M)$. Then*

$$L[\varphi[h]] = \bigcup_{b \in B} \bigcup_{y \in \mathfrak{g}/2\varphi(b,M)} (b + ye_1)C.$$

3.3 Lemma. *Let the notation be the same as in Theorem 3.2. We let $q \in \mathfrak{g} \cap F^\times$. Assume $r \geq 2$. If there are a finite number of elements $x_0, \cdots, x_\tau$ of M such that*

$$M[q] = \sqcup_{i=0}^{\tau} x_i C(M) \text{ and } \varphi(x_i, M) = 2^{-1}\mathfrak{p}^i, \tag{3.4}$$

then we have $L[q] = \sqcup_{i=0}^{\tau} x_i C$ and $\varphi(x_i, L) = 2^{-1}\mathfrak{p}^i$.

Proof. From (3.4) and Theorem 3.2(4),

$$L[q] = \bigcup_{i=0}^{\tau} \bigcup_{y \in \mathfrak{g}/\mathfrak{p}^i} (x_i + ye_1)C. \tag{3.5}$$

We fix $0 \leq i \leq \tau$. By (2.5), (2.6), (3.1), and (3.4),

$$\varphi(x_i + ye_1, L) = \varphi(x_i, M) + 2^{-1}y\mathfrak{g} = \begin{cases} 2^{-1}\mathfrak{p}^i & \text{if } y \in \mathfrak{p}^i, \\ 2^{-1}y\mathfrak{g} & \text{if } y \notin \mathfrak{p}^i. \end{cases}$$

From this and [IQD, Theorem 1.3],

$$(x_i + ye_1)C = L[q, \varphi(x_i + ye_1, L)] = \begin{cases} L[q, 2^{-1}\mathfrak{p}^i] & \text{if } y \in \mathfrak{p}^i, \\ L[q, 2^{-1}y\mathfrak{g}] & \text{if } y \notin \mathfrak{p}^i. \end{cases} \tag{3.6}$$

For $y \in \mathfrak{g}$ such that $y \notin \mathfrak{p}^i$, if $y\mathfrak{g} = \mathfrak{p}^j$ then $0 \leq j \leq i-1$. Thus we see that $\cup_{y \in \mathfrak{g}/\mathfrak{p}^i}(x_i + ye_1)C = \sqcup_{j=0}^{i} L[q, 2^{-1}\mathfrak{p}^j]$ and $L[q, 2^{-1}\mathfrak{p}^i] = x_iC$ by (3.6). From this and (3.5) we obtain

$$L[q] = \bigcup_{i=0}^{\tau} \left[\bigsqcup_{j=0}^{i} L[q, 2^{-1}\mathfrak{p}^j] \right] = \bigsqcup_{i=0}^{\tau} L[q, 2^{-1}\mathfrak{p}^i] = \bigsqcup_{i=0}^{\tau} x_iC.$$

Clearly $\varphi(x_i, L) = 2^{-1}\mathfrak{p}^i$ by (2.5), (2.6), (3.1), and (3.4). This completes the proof. $\square$

3.4 Lemma. *In the Witt decomposition of V of* (2.4)*, let N be as in* (2.7)*. Let q be an element of $\mathfrak{g} \cap F^\times$ and ξ as in Notation. Let t and c be as in* §2.2 *and* §2.3*, respectively. Then we obtain the following assertions:*

(1) *If $t = 1$, then $N[q] \neq \emptyset$ if and only if $\xi(cq) = 1$.*
(2) *Assume $t = 2$. Let K, $\mathfrak{r}$, and δ be as in* §2.3(II)*. Let $\nu \in \mathbf{Z}$ such that $q\mathfrak{g} = \mathfrak{p}^\nu$. Then $N[q] \neq \emptyset$ if and only if $c^{-1}q \in N_{K/F}(\mathfrak{r})$. Moreover if K is unramified over F, then this is the case if and only if $\nu \equiv \delta \pmod 2$.*
(3) *If $t = 3$, then $N[q] \neq \emptyset$ if and only if $\xi(-cq) \neq 1$.*
(4) *If $t = 4$, then we have $N[q] \neq \emptyset$ for all $q \in \mathfrak{g} \cap F^\times$.*
(5) *Let L be a maximal lattice in V and r as in* (2.4)*. If $r > 0$, then we have $L[q] \neq \emptyset$ for all $q \in \mathfrak{g} \cap F^\times$.*

Proof. We may assume that:

if $t = 1$, then $Z = F$, $N = \mathfrak{g}$, and $\varphi[x] = cx^2$ for $x \in F$;
if $t = 2$, then $Z = K$, $N = \mathfrak{r}$, and $\varphi[x] = cN_{K/F}(x)$ for $x \in K$;
if $t = 3$, then $Z = T$, $N = T \cap \mathfrak{P}^{-\delta}$, and $\varphi[x] = cN_{B/F}(x) = -cx^2$ for $x \in T$;
if $t = 4$, then $Z = B$, $N = \mathfrak{O}$, and $\varphi[x] = N_{B/F}(x)$ for $x \in B$

in (2.4); see §2.3. Then (1) and the first statement of (2) are trivial. We prove the second assertion of (2). Assume that $t = 2$ and K is unramified over F, then $\pi\mathfrak{r} = \mathfrak{q}$ and $N_{K/F}(\mathfrak{r}^\times) = \mathfrak{g}^\times$ by [BNT, Chapter VIII, Proposition 3]. Here $\mathfrak{q}$ is the maximal ideal of $\mathfrak{r}$. From these, we obtain the second assertion of (2). Assume $t = 3$. Noticing that B is division, the "only if"-part of (3) is immediate. If $\xi(-cq) \neq 1$, then $F(\sqrt{-c^{-1}q})$ is a quadratic extension of F, and hence there exists $z \in B$ such that $z \notin F$ and $z^2 = -c^{-1}q$ by [AQC, Proposition 5.15(ii)]. We easily see that $z \in T \cap \mathfrak{P}^{-\delta}$, and hence $N[q] \neq \emptyset$. Assume $t = 4$. Then we see that $N_{B/F}(\mathfrak{O}) = \mathfrak{g}$ from [AQC, Theorem 5.13] and [AQC, Proposition 5.15(i)]. This implies (4). Finally we prove (5). Assume $r > 0$. Since L can be represented as in (2.4), we have $f_1 + qe_1 \in L[q]$ for every $q \in \mathfrak{g} \cap F^\times$ with e_1 and f_1 in (2.4). This completes the proof. $\square$

Now, our first main result in this paper can be stated as follows:

3.5 Theorem. *Let L be a maximal lattice in V and put $C = C(L)$ as in Theorem* 3.2*. Let ξ be as in Notation. Let $q \in \mathfrak{g} \cap F^\times$ and $\nu \in \mathbf{Z}$ such that*

$q\mathfrak{g} = \mathfrak{p}^\nu$. *Let* $\kappa \in \mathbf{Z}$ *such that* $2\mathfrak{g} = \mathfrak{p}^\kappa$. *Let* r, t, e_r, f_r, *and* N *be as in* §2.2. *For* $0 \le i \in \mathbf{Z}$ *and* $x \in N$, *put*

$$(3.7)\qquad h_{i,x} = x + \pi^i e_r,\ k_{i,x} = \pi^i f_r + x + \frac{q - \varphi[x]}{\pi^i} e_r,\ \ell_i = \pi^i f_r + q\pi^{-i} e_r.$$

Then we have

$$(3.8)\qquad L[q] = \bigsqcup_{u \in R} uC = \begin{cases} L[q, 2^{-1}\mathfrak{p}^{\tau(q)}] & \text{if } r = 0, \\ \bigsqcup_{i=0}^{\tau(q)} L[q, 2^{-1}\mathfrak{p}^i] & \text{if } r \ge 1. \end{cases}$$

Here the set R *and the index* $\tau(q)$ *are defined as follows:*
(i) *Suppose* $t = 0$ *and* $r \ge 1$. *Then*

$$R = \begin{cases} \{\ell_i\}_{i=0}^{\nu} & \text{if } r = 1, \\ \{\ell_i\}_{i=0}^{\tau(q)} & \text{if } r \ge 2, \end{cases}$$

$$(3.9)\qquad \tau(q) = [\nu/2].$$

Moreover

$$(3.10)\qquad L[q, 2^{-1}\mathfrak{p}^i] = \begin{cases} \ell_i C \sqcup \ell_{\nu-i} C & \text{if } r = 1 \text{ and } 0 \le i < \nu/2, \\ \ell_{\nu/2} C & \text{if } r = 1,\ \nu \in 2\mathbf{Z}, \text{ and } i = \nu/2, \\ \ell_i C & \text{if } r \ge 2. \end{cases}$$

(ii) *Suppose* $t = 1$. *Let* c *be as in* (2.9) *and* δ *as in* (2.10). *Let us define an integer* $d \in \mathbf{Z}$ *as follows:* $D_{F(\sqrt{cq})/F} = \mathfrak{p}^d$ *when* $\xi(cq) = 0$ *(in the ordinary sense) and* $d = 1$ *when* $\xi(cq) = -1$ *(This is only for a simplification of the following statements* (3.11) *and* (3.12)*). When* $\xi(cq) = 1$, *we take any element* y *of* $N[q]$ *and fix it (By Lemma* 3.4(1), $N[q] \ne \emptyset$*). When* $2 \in \mathfrak{p}$, $\xi(cq) \ne 1$, *and* $\nu \equiv \delta \pmod 2$, *take any element* z *of* $N[sq]$ *and fix it, with*

$$(3.11)\qquad s \in 1 + \pi^{2\kappa+1-d}\mathfrak{g}^\times \text{ such that } c^{-1}q\pi^{\delta-\nu} \in s^{-1}\mathfrak{g}^{\times 2}.$$

(As for the existence of s *and* z, *see* (4.30) *and* (4.31), *respectively.) Then* R *and* $\tau(q)$ *are given as follows:*

$$R = \begin{cases} \{\pm y\} & \text{if } r = 0 \text{ and } \xi(cq) = 1, \\ \{y\} \sqcup \{h_{i,y}\}_{i=0}^{\tau(q)-1} & \text{if } r \ge 1 \text{ and } \xi(cq) = 1, \\ \{k_{i,z}\}_{i=0}^{\tau(q)} & \text{if } r \ge 1,\ \xi(cq) \ne 1, \\ & \qquad \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \{\ell_i\}_{i=0}^{\tau(q)} & \text{otherwise}, \end{cases}$$

$$(3.12)\qquad \tau(q) = \begin{cases} \kappa + \frac{\nu+\delta}{2} & \text{if } \xi(cq) = 1, \\ \kappa + \left[\frac{\nu+1-d}{2}\right] & \text{if } \xi(cq) \ne 1,\ \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \left[\frac{\nu}{2}\right] & \text{otherwise}. \end{cases}$$

Moreover

(3.13)

$$L[q,2^{-1}\mathfrak{p}^i] = \begin{cases} yC \sqcup (-y)C & \text{if } r = 0,\ \xi(cq) = 1,\ \text{and } i = \tau(q), \\ yC & \text{if } r \geq 1,\ \xi(cq) = 1,\ \text{and } i = \tau(q), \\ h_{i,y}C & \text{if } r \geq 1,\ \xi(cq) = 1,\ \text{and } i < \tau(q), \\ k_{i,z}C & \text{if } r \geq 1,\ \xi(cq) \neq 1, \\ & \quad \nu \equiv \delta \pmod 2,\ \text{and } 2 \in \mathfrak{p}, \\ \ell_i C & \text{otherwise.} \end{cases}$$

(iii) *Suppose* $t = 2$. *Let* c *and* δ *be as in* (2.12) *and* (2.13), *respectively. Let* K *and* $\mathfrak{r}$ *be as in* §2.3(II). *Let* $\mathfrak{d}$ *be the different of* K *relative to* F. *Let* $d \in \mathbf{Z}$ *such that* $D_{K/F} = \mathfrak{p}^d$ *when* $\mathfrak{d} \neq \mathfrak{r}$. *Put* $d = 1$ *when* $\mathfrak{d} = \mathfrak{r}$ *(This is the same simplification as in* (ii)*). When* $c^{-1}q \in N_{K/F}(\mathfrak{r})$, *we take any element* y *of* $N[q]$ *and fix it (By Lemma* 3.4(2), $N[q] \neq \emptyset$*). When* $c^{-1}q \notin N_{K/F}(\mathfrak{r})$ *and* $d > 1$, *we take any element* z *of* $N[sq]$ *and fix it, with*

$$s \in 1 + \pi^{d-1}\mathfrak{g}^\times \text{ such that } c^{-1}q\pi^{-\nu} \in s^{-1}N_{K/F}(\mathfrak{r}^\times). \tag{3.14}$$

(As for the existence of s *and* z, *see* (4.32) *and* (4.33), *respectively.) Then* R *and* $\tau(q)$ *are given as follows:*

$$R = \begin{cases} \{y\} & \text{if } r = 0 \text{ and } c^{-1}q \in N_{K/F}(\mathfrak{r}), \\ \{y\} \sqcup \{h_{i,y}\}_{i=0}^{\tau(q)-1} & \text{if } r \geq 1 \text{ and } c^{-1}q \in N_{K/F}(\mathfrak{r}), \\ \{k_{i,z}\}_{i=0}^{\tau(q)} & \text{if } r \geq 1,\ c^{-1}q \notin N_{K/F}(\mathfrak{r}),\ \text{and } d > 1, \\ \{\ell_i\}_{i=0}^{\tau(q)} & \text{otherwise,} \end{cases}$$

$$\tau(q) = \begin{cases} \frac{\nu+\delta}{2} & \text{if } c^{-1}q \in N_{K/F}(\mathfrak{r}) \text{ and } \mathfrak{d} = \mathfrak{r}, \\ \left[\frac{\nu+d}{2}\right] & \text{if } c^{-1}q \in N_{K/F}(\mathfrak{r}) \text{ and } \mathfrak{d} \neq \mathfrak{r}, \\ \left[\frac{\nu+d-1}{2}\right] & \text{otherwise.} \end{cases} \tag{3.15}$$

Moreover

$$L[q,2^{-1}\mathfrak{p}^i] = \begin{cases} yC & \text{if } c^{-1}q \in N_{K/F}(\mathfrak{r}) \text{ and } i = \tau(q), \\ h_{i,y}C & \text{if } c^{-1}q \in N_{K/F}(\mathfrak{r}) \text{ and } i < \tau(q), \\ k_{i,z}C & \text{if } c^{-1}q \notin N_{K/F}(\mathfrak{r}) \text{ and } d > 1, \\ \ell_i C & \text{otherwise.} \end{cases} \tag{3.16}$$

(iv) *Suppose* $t = 3$. *Let* c *and* δ *be as in* (2.14) *and* (2.15), *respectively. When* $\xi(-cq) \neq 1$, *we take any element* y *of* $N[q]$ *and fix it (By Lemma* 3.4(3), $N[q] \neq \emptyset$*). When* $\xi(-cq) = 1$ *and* $2 \in \mathfrak{p}$, *we take any element* z *of* $N[sq]$ *and fix it, with*

$$s \in 1 + 4\mathfrak{g} \text{ such that } s \notin \mathfrak{g}^{\times 2}. \tag{3.17}$$

(As for the existence of s and z, see (4.34) *and* (4.35)*, respectively.) Then R and $\tau(q)$ are given as follows:*

$$R = \begin{cases} \{y\} & \text{if } r = 0 \text{ and } \xi(-cq) \neq 1, \\ \{y\} \sqcup \{h_{i,y}\}_{i=0}^{\tau(q)-1} & \text{if } r \geq 1 \text{ and } \xi(-cq) \neq 1, \\ \{k_{i,z}\}_{i=0}^{\tau(q)} & \text{if } r \geq 1,\ \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}, \\ \{\ell_i\}_{i=0}^{\tau(q)} & \text{if } r \geq 1,\ \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{g}^\times, \end{cases}$$

$$\tau(q) = \begin{cases} \kappa + \left[\frac{\nu}{2}\right] & \text{if } \xi(-cq) = 1, \\ \frac{\nu-\delta+1}{2} & \text{if } \xi(-cq) \neq 1 \text{ and } \nu \not\equiv \delta \pmod 2, \\ \kappa + 1 + \frac{\nu-\delta-d}{2} & \text{if } \xi(-cq) = 0,\ \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \kappa + \frac{\nu+\delta}{2} & \text{otherwise,} \end{cases} \tag{3.18}$$

where $d \in \mathbf{Z}$ such that $D_{F(\sqrt{-cq})/F} = \mathfrak{p}^d$. Moreover

$$L[q, 2^{-1}\mathfrak{p}^i] = \begin{cases} yC & \text{if } \xi(-cq) \neq 1 \text{ and } i = \tau(q), \\ h_{i,y}C & \text{if } \xi(-cq) \neq 1 \text{ and } i < \tau(q), \\ k_{i,z}C & \text{if } \xi(-cq) = 1 \text{ and } 2 \in \mathfrak{p}, \\ \ell_i C & \text{if } \xi(-cq) = 1 \text{ and } 2 \in \mathfrak{g}^\times. \end{cases} \tag{3.19}$$

(v) *Suppose $t = 4$. Take any element y of $N[q]$ and fix it. Then R and $\tau(q)$ are given as follows:*

$$R = \begin{cases} \{y\} & \text{if } r = 0, \\ \{y\} \sqcup \{h_{i,y}\}_{i=0}^{\tau(q)-1} & \text{if } r \geq 1, \end{cases}$$

$$\tau(q) = [(\nu+1)/2]. \tag{3.20}$$

Moreover

$$L[q, 2^{-1}\mathfrak{p}^i] = \begin{cases} yC & \text{if } i = \tau(q), \\ h_{i,y}C & \text{if } i < \tau(q). \end{cases} \tag{3.21}$$

The proof of this theorem will be given in the following Section 4. Here we insert one elementary lemma:

3.6 Lemma. *Let F be a local field and L a maximal lattice in V. Let $\kappa \in \mathbf{Z}$ such that $2\mathfrak{g} = \mathfrak{p}^\kappa$. Then for $q \in \mathfrak{g}$ and $i \in \mathbf{Z}$, we have $L[q, \mathfrak{p}^i] \subset L[q]$ if and only if $i \geq -\kappa$.*

Proof. From (2.2), clearly $i \geq -\kappa$ if and only if $L[q, \mathfrak{p}^i] \subset \tilde{L}[q]$. Here [AQC, Lemma 6.2(3)] implies $\tilde{L}[q] = L[q]$. This proves the lemma. ☐

3.7 Corollary. *Let the notation be the same as in Theorem* 3.5*. Assume $L[q] \neq \emptyset$ for $q \in \mathfrak{g} \cap F^\times$. Then for every $i \in \mathbf{Z}$,*

$$L[q, 2^{-1}\mathfrak{p}^i] \neq \emptyset \iff \begin{cases} i = \tau(q) & \text{if } n = t, \\ i \leq \tau(q) & \text{otherwise.} \end{cases}$$

Proof. For $0 \leq i \in \mathbf{Z}$, the result follows from Theorem 3.5 and Lemma 3.6. Assume $i < 0$. Clearly $L[q, 2^{-1}\mathfrak{p}^i] = \pi^i \cdot L[\pi^{-2i}q, 2^{-1}\mathfrak{g}]$. Here Lemma 3.6 implies $L[\pi^{-2i}q, 2^{-1}\mathfrak{g}] \subset L[\pi^{-2i}q]$. Since $\pi^i \cdot L[\pi^{-2i}q] = (\pi^i L)[q] \supset L[q]$, we obtain $L[\pi^{-2i}q] \neq \emptyset$. Applying Theorem 3.5 to (V, φ), L, and $\pi^{-2i}q$, we find that if $n = t$ then $L[\pi^{-2i}q] = L[\pi^{-2i}q, 2^{-1}\mathfrak{p}^{\tau(\pi^{-2i}q)}]$ and $\tau(\pi^{-2i}q) = \tau(q) - i > 0$. Therefore $L[\pi^{-2i}q, 2^{-1}\mathfrak{g}] = \emptyset$, and hence $L[q, 2^{-1}\mathfrak{p}^i] = \emptyset$. If $n \neq t$, then $L[\pi^{-2i}q, 2^{-1}\mathfrak{g}] \neq \emptyset$ by Theorem 3.5, and hence $L[q, 2^{-1}\mathfrak{p}^i] \neq \emptyset$. This completes the proof. □

4 PROOF OF THEOREM 3.5

4.1. We first prove Theorem 3.5(i). Assume $t = 0$. Then $L[q] \neq \emptyset$ for all $q \in \mathfrak{g} \cap F^\times$ by Lemma 3.4(5).
First suppose $r = 1$. Then $L = \mathfrak{g}f_1 + \mathfrak{g}e_1$ by (2.4). We obtain

$$L[q] = \bigsqcup_{i=0}^{\nu} \ell_i C \tag{4.1}$$

by Theorem 3.2(2) with ℓ_i in (3.7). We have clearly

$$\varphi(\ell_i, L) = 2^{-1}\pi^i\mathfrak{g} + 2^{-1}q\pi^{-i}\mathfrak{g} = \begin{cases} 2^{-1}\mathfrak{p}^i & \text{if } 0 \leq i \leq [\nu/2], \\ 2^{-1}\mathfrak{p}^{\nu-i} & \text{if } i > [\nu/2] \end{cases} \tag{4.2}$$

from (2.5). Assume $\nu \in 2\mathbf{Z}$. Then

$$\varphi(\ell_i, L) = \varphi(\ell_{\nu-i}, L) = 2^{-1}\mathfrak{p}^i \tag{4.3}$$

for $0 \leq i \leq (\nu-2)/2$ and $\varphi(\ell_{\nu/2}, L) = 2^{-1}\mathfrak{p}^{\nu/2}$ by (4.2). Thus $\ell_i C \sqcup \ell_{\nu-i} C \subset L[q, 2^{-1}\mathfrak{p}^i]$ for $0 \leq i \leq (\nu-2)/2$ and $\ell_{\nu/2} C \subset L[q, 2^{-1}\mathfrak{p}^{\nu/2}]$. On the other hand, we have $L[q, 2^{-1}\mathfrak{p}^i] \subset L[q]$ for $0 \leq i \leq \nu/2$ by Lemma 3.6. Hence $\ell_i C \sqcup \ell_{\nu-i} C = L[q, 2^{-1}\mathfrak{p}^i]$ for $0 \leq i \leq (\nu-2)/2$ and $\ell_{\nu/2} C = L[q, 2^{-1}\mathfrak{p}^{\nu/2}]$. From this and (4.1) we obtain the assertion in the case $r = 1$, $t = 0$, and $\nu \in 2\mathbf{Z}$. Next assume $\nu \notin 2\mathbf{Z}$. Then

$$\varphi(\ell_i, L) = \varphi(\ell_{\nu-i}, L) = 2^{-1}\mathfrak{p}^i \tag{4.4}$$

for $0 \leq i \leq (\nu-1)/2$. Thus $\ell_i C \sqcup \ell_{\nu-i} C = L[q, 2^{-1}\mathfrak{p}^i]$ for $0 \leq i \leq (\nu-1)/2$, in the same manner as in the case $\nu \in 2\mathbf{Z}$. This proves the assertion when $r = 1$ and $t = 0$.
Next suppose $r = 2$. Then $L = \mathfrak{g}f_1 + M + \mathfrak{g}e_1$ by (3.1). We obtain

$$\emptyset \neq M[q] = \sqcup_{i=0}^{\nu} \ell_i C(M) \tag{4.5}$$

by Theorem 3.2(2) and Lemma 3.4(5). In this case we can not apply Lemma 3.3 since we have (4.3) and (4.4) in the notation of (4.1). By (4.5) and Theorem 3.2(4),

$$L[q] = \bigcup_{i=0}^{\nu} \bigcup_{a \in \mathfrak{g}/2\varphi(\ell_i, M)} (\ell_i + ae_1)C.$$

Since

$$2\varphi(\ell_i, M) = \begin{cases} \mathfrak{p}^i & \text{if } 0 \le i \le [\nu/2], \\ \mathfrak{p}^{\nu-i} & \text{if } i > [\nu/2] \end{cases}$$

by (4.2), we have

$$L[q] = \Big[\bigcup_{i=0}^{[\nu/2]} \bigcup_{a\in\mathfrak{g}/\mathfrak{p}^i} (\ell_i + ae_1)C\Big] \bigcup \Big[\bigcup_{j>[\nu/2]}^{\nu} \bigcup_{b\in\mathfrak{g}/\mathfrak{p}^{\nu-j}} (\ell_j + be_1)C\Big]. \tag{4.6}$$

For $0 \le i \le [\nu/2]$ and $a \in \mathfrak{g}/\mathfrak{p}^i$,

$$\varphi(\ell_i + ae_1, L) = \varphi(\ell_i, M) + 2^{-1}a\mathfrak{g} = \begin{cases} 2^{-1}\mathfrak{p}^i & \text{if } a \in \mathfrak{p}^i, \\ 2^{-1}a\mathfrak{g} & \text{if } a \notin \mathfrak{p}^i \end{cases}$$

by (2.5) and (3.1). Therefore by [IQD, Theorem 1.3],

$$(\ell_i + ae_1)C = L[q, \varphi(\ell_i + ae_1, L)] = \begin{cases} L[q, 2^{-1}\mathfrak{p}^i] & \text{if } a \in \mathfrak{p}^i, \\ L[q, 2^{-1}a\mathfrak{g}] & \text{if } a \notin \mathfrak{p}^i. \end{cases} \tag{4.7}$$

Similarly we have

$$(\ell_j + be_1)C = \begin{cases} L[q, 2^{-1}\mathfrak{p}^{\nu-j}] & \text{if } b \in \mathfrak{p}^{\nu-j}, \\ L[q, 2^{-1}b\mathfrak{g}] & \text{if } b \notin \mathfrak{p}^{\nu-j} \end{cases} \tag{4.8}$$

for $j > [\nu/2]$ and $b \in \mathfrak{g}/\mathfrak{p}^{\nu-j}$. From (4.7) and (4.8), the argument in the proof of Lemma 3.3 shows that

$$\bigcup_{i=0}^{[\nu/2]} \bigcup_{a\in\mathfrak{g}/\mathfrak{p}^i} (\ell_i + ae_1)C = \bigsqcup_{i=0}^{[\nu/2]} \ell_i C, \quad \ell_i C = L[q, 2^{-1}\mathfrak{p}^i], \tag{4.9}$$

$$\bigcup_{j>[\nu/2]}^{\nu} \bigcup_{b\in\mathfrak{g}/\mathfrak{p}^{\nu-j}} (\ell_j + be_1)C = \bigsqcup_{j>[\nu/2]}^{\nu} \ell_j C, \quad \ell_j C = L[q, 2^{-1}\mathfrak{p}^{\nu-j}]. \tag{4.10}$$

Combining (4.6), (4.9), and (4.10), we have

$$L[q] = \Big(\bigsqcup_{i=0}^{[\nu/2]} \ell_i C\Big) \cup \Big(\bigsqcup_{j>[\nu/2]}^{\nu} \ell_j C\Big) = \bigsqcup_{i=0}^{[\nu/2]} L[q, 2^{-1}\mathfrak{p}^i] = \bigsqcup_{i=0}^{[\nu/2]} \ell_i C$$

and $L[q, 2^{-1}\mathfrak{p}^i] = \ell_i C$. This proves our theorem in the case $r = 2$ and $t = 0$. As for the case $r \ge 3$, we apply (repeatedly, if necessary) Lemma 3.3 and [IQD, Theorem 1.3] to this case, we can reduce the proof to the case $r = 2$. This completes the proof of (i).

4.2 LEMMA. *Let F be a local field. Assume $2 \in \mathfrak{p}$ and let $\kappa \in \mathbf{Z}$ such that $2\mathfrak{g} = \mathfrak{p}^\kappa$. Let ξ be as in Notation. Put*

$$\varepsilon(a) = \max(\{e \in \mathbf{Z} \mid e \leq 2\kappa + 1 \text{ and } a \in (1 + \mathfrak{p}^e)\mathfrak{g}^{\times 2}\}) \tag{4.11}$$

for $a \in \mathfrak{g}^\times$. Then we obtain the following assertions:

(1) *For $a \in \mathfrak{g}^\times$,*

$$\varepsilon(a) = \begin{cases} 2\kappa + 1 - d & \text{if } \xi(a) = 0, \\ 2\kappa & \text{if } \xi(a) = -1, \\ 2\kappa + 1 & \text{if } \xi(a) = 1, \end{cases} \tag{4.12}$$

where $d \in \mathbf{Z}$ such that $D_{F(\sqrt{a})/F} = \mathfrak{p}^d$.
(2) *If $\xi(a) = 0$, then we have $2\kappa > \varepsilon(a) \notin 2\mathbf{Z}$.*
(3) *If $0 < \ell < 2\kappa$ and $\ell \in \mathbf{Z}$, $\notin 2\mathbf{Z}$, then $\mathfrak{g}^{\times 2} \cap (1 + \pi^\ell \mathfrak{g}^\times) = \emptyset$.*
(4) *If $a \in (1 + \pi^\ell \mathfrak{g}^\times)\mathfrak{g}^{\times 2}$ with $0 < \ell \in \mathbf{Z}$, $\notin 2\mathbf{Z}$ and $\varepsilon(a) < 2\kappa$, then $\varepsilon(a) = \ell$.*
(5) *If $a \in (1 + \pi^\ell \mathfrak{g}^\times)\mathfrak{g}^{\times 2}$ with $0 < \ell \in \mathbf{Z}$, $\notin 2\mathbf{Z}$ and $\varepsilon(a) = 2\kappa + 1$, then $\varepsilon(a) \leq \ell$.*

Proof. Assertions (1) and (2) are in [NRQ, Lemma 3.5]. (3): If there exists an element $b \in \mathfrak{g}^\times$ such that $b^2 \in 1 + \pi^\ell \mathfrak{g}^\times$, then $b \in Z_\ell$. Here $Z_\ell = \{x \in \mathfrak{g}^\times \mid x^2 - 1 \in \mathfrak{p}^\ell\}$ as in [NRQ, §3.4]. By [NRQ, (3.5.1)], $Z_\ell = 1 + \mathfrak{p}^{(\ell+1)/2}$, and hence we can take $y \in \mathfrak{g}$ such that $b = 1 + \pi^{(\ell+1)/2} y$. Then $b^2 = 1 + \pi^{\ell+1} y(2\pi^{-(\ell+1)/2} + y) \in 1 + \mathfrak{p}^{\ell+1}$ since $2^{-1}(\ell+1) \leq \kappa$. This gives a contradiction. Thus we obtain (3). (4): We find $\ell \leq \varepsilon(a)$ from (4.11), (4.12), and [NRQ, Lemma 3.2(1)]. Clearly

$$(1 + \pi^\ell \mathfrak{g}^\times)\mathfrak{g}^{\times 2} \cap (1 + \mathfrak{p}^{\varepsilon(a)})\mathfrak{g}^{\times 2} \neq \emptyset. \tag{4.13}$$

If $\ell < \varepsilon(a)$, then (4.13) contradicts (3) settled above, and hence $\ell = \varepsilon(a)$. (5): By (4.12), we have $\xi(a) = 1$. Thus

$$\mathfrak{g}^{\times 2} \cap (1 + \pi^\ell \mathfrak{g}^\times) \neq \emptyset. \tag{4.14}$$

If $\ell < \varepsilon(a) = 2\kappa + 1$, then (4.14) contradicts (3). This completes the proof. □

4.3. Now we prove (ii), (iii), (iv), and (v) of Theorem 3.5. We may assume that:

if $t = 1$, then $Z = F$, $N = \mathfrak{g}$, and $\varphi[x] = cx^2$ for $x \in F$;
if $t = 2$, then $Z = K$, $N = \mathfrak{r}$, and $\varphi[x] = cN_{K/F}(x)$ for $x \in K$;
if $t = 3$, then $Z = T$, $N = \mathfrak{g}v + \mathfrak{r}\omega^{1-2\delta}$, and $\varphi[x] = cN_{B/F}(x)$ for $x \in T$;
if $t = 4$, then $Z = B$, $N = \mathfrak{O}$, and $\varphi[x] = N_{B/F}(x)$ for $x \in B$.

Then for $x, w \in Z$,

$$\varphi(x, w) = \begin{cases} cxw & \text{if } t = 1, \\ 2^{-1} c Tr_{K/F}(xw^\rho) & \text{if } t = 2, \\ 2^{-1} c Tr_{B/F}(xw^\iota) & \text{if } t = 3, \\ 2^{-1} Tr_{B/F}(xw^\iota) & \text{if } t = 4. \end{cases} \tag{4.15}$$

Here $\rho \in Gal(K/F)$ such that $\rho \neq 1$. In this §4.3 we prove the theorem in the case $r = 0$ and $t > 0$. Note that $L = N$ in this case. If $L[q] \neq \emptyset$, then

$$L[q] = \begin{cases} yC \sqcup (-y)C & \text{if } t = 1, \\ yC & \text{otherwise} \end{cases} \tag{4.16}$$

by Theorem 3.2(1). Here, y is any element of $L[q]$ and fix it until the end of §4.3. This proves the first equality of (3.8) in this case. From Lemma 3.6 and (4.16),

$$L[q] = L[q, \varphi(y, L)] \tag{4.17}$$

for $1 \leq t \leq 4$. Note that $\varphi(y, L) \subset 2^{-1}\mathfrak{g}$ since L is an integral lattice in V. To prove the second equality of (3.8) we determine the ideal $\varphi(y, L)$ as the next step.

(4.18) We let μ denote the normalized order function of F.

First suppose $t = 1$, then $C = \{1\}$. Here Lemma 3.4(1) implies that $L[q] \neq \emptyset$ if and only if $\xi(cq) = 1$. Since $y^2 = c^{-1}q$, we have $\varphi(y, L) = cy\mathfrak{g} = \mathfrak{p}^{(\nu+\delta)/2}$ by (4.15).

Next suppose $t = 2$. We have $L[q] \neq \emptyset$ if and only if $c^{-1}q \in N_{K/F}(\mathfrak{r})$ by Lemma 3.4(2). From [BNT, Chapter VIII, Propositon 4] and (4.15), we see that

$$\varphi(y, L) = 2^{-1}cTr_{K/F}(y\mathfrak{r}) = \begin{cases} 2^{-1}\mathfrak{p}^{(\nu+\delta)/2} & \text{if } \mathfrak{d} = \mathfrak{r}, \\ 2^{-1}\mathfrak{p}^{[(\nu+d)/2]} & \text{if } \mathfrak{d} \neq \mathfrak{r}. \end{cases}$$

Note that we take $c \in \mathfrak{g}^\times$ if K is ramified over F; see §2.3.

Suppose $t = 3$. By Lemma 3.4(3),

$$L[q] \neq \emptyset \text{ if and only if } \xi(-cq) \neq 1. \tag{4.19}$$

Take $m \in \mathbf{Z}$ such that $\varphi(y, L) = 2^{-1}\mathfrak{p}^m$. Let us determine m. Let μ_K be the normalized order function of K. Since $L = \mathfrak{g}v + \mathfrak{r}\omega^{1-2\delta} = v(\mathfrak{g} + \mathfrak{r}\omega^{1-2\delta})$, we can put $y = v(a + b\omega^{1-2\delta})$ with $a \in \mathfrak{g}$ and $b \in \mathfrak{r}$. Then by (2.18), $\varphi(y, L) = 2^{-1}c(2a\mathfrak{g} + \omega^{2(1-2\delta)}Tr_{K/F}(b\mathfrak{r}))$, and hence

$$m = \min(\kappa + \delta + \mu(a), 1 + \mu_K(b) - \delta). \tag{4.20}$$

We have also

$$q = \varphi[y] = -cv^2(a^2 - \omega^{2(1-2\delta)}N_{K/F}(b)) \tag{4.21}$$

by (2.17), and hence

$$\nu - \delta = \min(2\mu(a), 1 + 2(\mu_K(b) - \delta)). \tag{4.22}$$

Assume $\nu \not\equiv \delta \pmod 2$. Then $\nu - \delta = 1 + 2(\mu_K(b) - \delta) < 2\mu(a)$ by (4.22), and hence $2^{-1}(\nu-\delta+1) = 1+\mu_K(b)-\delta \le \kappa+\delta+\mu(a)$. Thus we find $m = 2^{-1}(\nu-\delta+1)$ by (4.20). Next assume $\nu \equiv \delta \pmod 2$. Then $\nu-\delta = 2\mu(a) < 1+2(\mu_K(b)-\delta)$ by (4.22). If $2 \in \mathfrak{g}^\times$, then $\kappa + 2^{-1}(\nu + \delta) = \kappa + \delta + \mu(a) \le 1 + \mu_K(b) - \delta$, and hence $m = \kappa + 2^{-1}(\nu + \delta)$ from (4.20). If $2 \in \mathfrak{p}$, then Lemma 4.2 implies $\varepsilon(-c^{-1}q\pi^{\delta-\nu}) \le 2\kappa$ since $\xi(-c^{-1}q\pi^{\delta-\nu}) \ne 1$ by (4.19). Put $\beta = -c^{-1}q\pi^{\delta-\nu}$, then

$$\varepsilon(v^{-2}\beta) = \begin{cases} \varepsilon(\beta) & \text{if } \varepsilon(\beta) < 2\kappa, \\ 2\kappa + 1 & \text{if } \varepsilon(\beta) = 2\kappa; \end{cases} \tag{4.23}$$

see the proof of [NRQ, Lemma 4.5]. By (4.21),

$$v^{-2}\beta = (\pi^{(\delta-\nu)/2}a)^2(1-\omega^{2(1-2\delta)}a^{-2}N_{K/F}(b)) \in (1-\omega^{2(1-2\delta)}a^{-2}N_{K/F}(b))\mathfrak{g}^{\times 2}. \tag{4.24}$$

Hence if $\varepsilon(\beta) < 2\kappa$, that is $\xi(-cq) = 0$ from Lemma 4.2, then Lemma 4.2(4) and (4.23) imply $\varepsilon(\beta) = 1 - 2\delta - 2\mu(a) + 2\mu_K(b)$, and hence $1 + \mu_K(b) - \delta = 2^{-1}(\varepsilon(\beta)+1)+2^{-1}(\nu-\delta) \le \kappa+\mu(a)+\delta$. Thus $m = 2^{-1}(\varepsilon(\beta)+1)+2^{-1}(\nu-\delta)$ from (4.20). Here Lemma 4.2(1) implies $\varepsilon(\beta) = 2\kappa + 1 - d$, where $d \in \mathbf{Z}$ such that $D_{F(\sqrt{-cq})/F} = \mathfrak{p}^d$. Therefore $m = \kappa+1+(\nu-\delta-d)/2$. If $\varepsilon(\beta) = 2\kappa$, then Lemma 4.2(5), (4.23), and (4.24) imply $2\kappa+1 \le 1-2\delta-2\mu(a)+2\mu_K(b)$, and hence $1 + \mu_K(b) - \delta \ge \kappa + \mu(a) + \delta$. Thus $m = \kappa + \mu(a) + \delta = \kappa + (\nu + \delta)/2$ from (4.20). Consequently we obtain

$$\varphi(y, L) = \begin{cases} 2^{-1}\mathfrak{p}^{(\nu-\delta+1)/2} & \text{if } \nu \not\equiv \delta \pmod 2, \\ \mathfrak{p}^{1+(\nu-\delta-d)/2} & \text{if } \nu \equiv \delta \pmod 2,\ 2 \in \mathfrak{p},\ \xi(-cq) = 0, \\ \mathfrak{p}^{(\nu+\delta)/2} & \text{otherwise} \end{cases} \tag{4.25}$$

under the assumption $t = 3$, $r = 0$, and $\xi(-cq) \ne 1$. Here $d \in \mathbf{Z}$ such that $D_{F(\sqrt{-cq})/F} = \mathfrak{p}^d$. We see the second equality of (3.8) by (4.17) and (4.25). Moreover combining this with (4.16), we obtain the theorem in the case $r = 0$ and $t = 3$.

Finally suppose $t = 4$. Then Lemma 3.4(4) implies $L[q] \ne \emptyset$ for every $q \in \mathfrak{g} \cap F^\times$. From [AQC, Theorem 5.9(2), (6), (7)] and (4.15), we see that

$$\varphi(y, L) = 2^{-1}Tr_{B/F}(\mathfrak{P}^{\mu(N_{B/F}(y))}) = 2^{-1}\mathfrak{p}^{[(\nu+1)/2]}, \tag{4.26}$$

where $\mathfrak{P} = \{x \in \mathfrak{O} \mid N_{B/F}(x) \in \mathfrak{p}\}$, with μ of (4.18). This completes the proof of our theorem in the case $r = 0$ and $t > 0$.

4.4. Here we prove the theorem in the case $r \ge 1$ and $t > 0$. First we note that when $r \ge 2$ we apply (repeatedly, if necessary) Lemma 3.3 and [IQD, Theorem 1.3] to this case, we can reduce the proof to the case $r = 1$.

Thus hereafter until the end of §4.7, we assume $r = 1$. Then $L = \mathfrak{g}f_1 + N + \mathfrak{g}e_1$ by (2.4). Assume $1 \le t \le 4$. We recall here Lemma 3.4. We know that $L[q] \ne \emptyset$

for all $q \in \mathfrak{g} \cap F^\times$ and

$$N[q] \neq \emptyset \Longleftrightarrow \begin{cases} \xi(cq) = 1 & \text{if } t = 1, \\ c^{-1}q \in N_{K/F}(\mathfrak{r}) & \text{if } t = 2, \\ \xi(-cq) \neq 1 & \text{if } t = 3. \end{cases} \tag{4.27}$$

When $t = 4$, we have $N[q] \neq \emptyset$ for every $q \in \mathfrak{g} \cap F^\times$.

4.5. In this § we prove the theorem in the case $r = 1$, $1 \le t \le 4$, and $N[q] \neq \emptyset$. Applying Theorem 3.2(1) and (4), we find

$$L[q] = \begin{cases} \Big[\bigcup_{a \in \mathfrak{g}/2\varphi(y,N)} (y + ae_1)C\Big] \cup \Big[\bigcup_{a \in \mathfrak{g}/2\varphi(-y,N)} (-y + ae_1)C\Big] & \text{if } t = 1, \\ \bigcup_{a \in \mathfrak{g}/2\varphi(y,N)} (y + ae_1)C & \text{otherwise,} \end{cases}$$

where y is any element of $N[q]$ and fix it. Since $\varphi(y+ae_1, L) = \varphi(-y+ae_1, L)$, we obtain $(y + ae_1)C = (-y + ae_1)C$ by [IQD, Theorem 1.3]. Thus $L[q] = \bigcup_{a \in \mathfrak{g}/2\varphi(y,N)} (y + ae_1)C$ for $1 \le t \le 4$. We have already obtained our theorem in the case $r = 0$ and $t > 0$. Thus $\varphi(y, N) = 2^{-1}\mathfrak{p}^{\tau(q)}$. Put simply $\tau = \tau(q)$. The same argument as in the proof of Lemma 3.3 shows that

$$(y + ae_1)C = \begin{cases} L[q, 2^{-1}\mathfrak{p}^\tau] & \text{if } a \in \mathfrak{p}^\tau, \\ L[q, 2^{-1}\mathfrak{p}^{\mu(a)}] & \text{if } a \notin \mathfrak{p}^\tau \end{cases}$$

with μ of (4.18). If $\tau \ge 1$, then $0 \le \mu(a) \le \tau - 1$ for $a \in \mathfrak{g}$ such that $a \notin \mathfrak{p}^\tau$. Thus

$$L[q] = \bigcup_{a \in \mathfrak{g}/\mathfrak{p}^\tau} (y + ae_1)C = \bigsqcup_{i=0}^{\tau} L[q, 2^{-1}\mathfrak{p}^i],$$

$L[q, 2^{-1}\mathfrak{p}^\tau] = yC$, and $L[q, 2^{-1}\mathfrak{p}^i] = (y + \pi^i e_1)C$ for $0 \le i \le \tau - 1$. If $\tau = 0$, then it is clear that $L[q] = yC = L[q, 2^{-1}\mathfrak{g}]$. This proves the theorem in the case $r = 1$, $t > 0$, and $N[q] \neq \emptyset$.

4.6. In §§4.6 and 4.7 we assume $r = 1$, $t > 0$, and $N[q] = \emptyset$. Then $1 \le t \le 3$ since $N[q] \neq \emptyset$ for all $q \in \mathfrak{g} \cap F^\times$ if $t = 4$. By Theorem 3.2(3),

$$L[q] = \bigcup_{i=0}^{\kappa_0 - 1} \bigcup_{b \in X_i(q)/\mathfrak{p}^i N} k_{i,b}C \tag{4.28}$$

with $k_{i,b}$ in (3.7). Let us determine κ_0 in this §4.6. With the notation of (3.2)

$$0 \in X_\nu(q) \tag{4.29}$$

since $q \in \mathfrak{p}^\nu$, and hence $\kappa_0 > \nu$ with the notation of (3.3). Suppose $t = 1$, then $\xi(cq) \neq 1$ by (4.27) and the assumption $N[q] = \emptyset$. First assume $2 \notin \mathfrak{p}$ or $\nu \not\equiv \delta \pmod 2$. If there exists $x \in X_{\nu+1}(q)$, then $x^2 \in c^{-1}q(1 + \mathfrak{p})$ by (3.2). This implies $\nu \equiv \delta \pmod 2$, and hence $2 \notin \mathfrak{p}$. Then by [NRQ, Lemma 3.2(1)], we have $1+\mathfrak{p} \subset \mathfrak{g}^{\times 2}$, which contradicts $\xi(cq) \neq 1$. Thus $\kappa_0 = \nu+1$ by (4.29). Next assume $2 \in \mathfrak{p}$ and $\nu \equiv \delta \pmod 2$. Then $\varepsilon(c^{-1}q\pi^{\delta-\nu}) \leq 2\kappa$ from $\xi(cq) \neq 1$ and Lemma 4.2. Hereafter we put $\varepsilon = \varepsilon(c^{-1}q\pi^{\delta-\nu})$. There exist

$$(4.30) \qquad s \in 1+\pi^{\varepsilon}\mathfrak{g}^{\times} \text{ and } \alpha \in \mathfrak{g}^{\times} \text{ such that } c^{-1}q\pi^{\delta-\nu} = s^{-1}\alpha^2$$

by (4.11). From this we have $c(\pi^{(\nu-\delta)/2}\alpha)^2 = sq$, and hence

$$(4.31) \qquad N[sq] \neq \emptyset.$$

Since $N[sq] \subset X_{\nu+\varepsilon}(q)$, we obtain $X_{\nu+\varepsilon}(q) \neq \emptyset$, and hence $\kappa_0 > \nu+\varepsilon$ in the notation of (3.3). If there exists $x \in X_{\nu+\varepsilon+1}(q)$, then we can take $a \in \mathfrak{p}^{\nu+\varepsilon+1}$ such that $cx^2 + a = q$. Thus $c^{-1}q\pi^{\delta-\nu} = (1+c^{-1}x^{-2}a)(\pi^{(\delta-\nu)/2}x)^2 \in (1+\mathfrak{p}^{\varepsilon+1})\mathfrak{g}^{\times 2}$, which contradicts (4.11). Hence $\kappa_0 = \nu+\varepsilon+1$. Moreover Lemma 4.2(1) implies that: if $\xi(cq) = -1$, then $\varepsilon = 2\kappa$, and hence $\kappa_0 = 2\kappa+\nu+1$; if $\xi(cq) = 0$ and $D_{F(\sqrt{cq})/F} = \mathfrak{p}^d$, then $\varepsilon = 2\kappa+1-d$, and hence $\kappa_0 = 2\kappa+\nu+2-d$.
Next suppose $t = 2$, then $c^{-1}q \notin N_{K/F}(\mathfrak{r})$ by (4.27). Let d be as in Theorem 3.5(iii). If $X_{\nu+d}(q) \neq \emptyset$, then $c^{-1}q \in N_{K/F}(\mathfrak{r})(1+\mathfrak{p}^d) \subset N_{K/F}(\mathfrak{r})$ by [BNT, Chapter VIII, Proposition 3] or the conductor-discriminant theorem according as $\mathfrak{d} = \mathfrak{r}$ or $\mathfrak{d} \neq \mathfrak{r}$. This contradicts $c^{-1}q \notin N_{K/F}(\mathfrak{r})$. Thus $\kappa_0 \leq \nu+d$. In particular if $\mathfrak{d} = \mathfrak{r}$ or $\mathfrak{q}$, that is $d = 1$, then $\kappa_0 = \nu+1$ from (4.29). Here $\mathfrak{q}$ is the maximal ideal of $\mathfrak{r}$. Assume $\mathfrak{d} = \mathfrak{q}^d$ and $d > 1$. Take a prime element π_K of K such that $N_{K/F}(\pi_K) = \pi$. We see that $2 \in \mathfrak{p}$ by [BNT, Chapter VIII, Corollary 3 of Proposition 7]. By local class field theory, we have $(1+\mathfrak{p}^{d-1})N_{K/F}(\mathfrak{r}^{\times}) = \mathfrak{g}^{\times}$. Thus there exist

$$(4.32) \qquad s \in 1+\pi^{d-1}\mathfrak{g}^{\times} \text{ and } \alpha \in \mathfrak{r}^{\times} \text{ such that } c^{-1}q\pi^{-\nu} = s^{-1}N_{K/F}(\alpha).$$

Note that $c \in \mathfrak{g}^{\times}$ since K is ramified over F; see §2.3. Then $cN_{K/F}(\pi_K^{\nu}\alpha) = sq$, and hence

$$(4.33) \qquad N[sq] \neq \emptyset.$$

We obtain $N[sq] \subset X_{\nu+d-1}(q)$ by the definition of s. Thus $\kappa_0 = \nu+d$.
Finally suppose $t = 3$. Then $\xi(-cq) = 1$ by (4.27), and hence $\nu \equiv \delta \pmod 2$. For $b \in \mathfrak{g}$ and $0 \leq m \in \mathbf{Z}$, put

$$Y_m(b) = \{y \in N \mid y^2 - b \in \mathfrak{p}^m\}$$

as in [NRQ, (4.1.3)]. Then $X_i(q) = \pi^{(\nu-\delta)/2}Y_{i-\nu}(-c^{-1}q\pi^{\delta-\nu})$ if $i > \nu$. The proof of [NRQ, Lemma 4.2(2)] shows that $Y_m(-c^{-1}q\pi^{\delta-\nu}) = \emptyset$ for $m \geq 2\kappa+1$ even for $c\mathfrak{g} = \mathfrak{p}$. Thus $\kappa_0 \leq \nu+2\kappa+1$. If $2 \in \mathfrak{g}^{\times}$, then $\kappa_0 = \nu+1$ by (4.29). Assume $2 \in \mathfrak{p}$. There exists

$$(4.34) \qquad s \in 1+4\mathfrak{g} \text{ such that } s \notin \mathfrak{g}^{\times 2}$$

by [NRQ, Lemma 3.2(1)], then $\xi(s) = -1$ from Lemma 4.2(1). Thus $\xi(-csq) = -1$, and hence, by Lemma 3.4(3),

$$N[sq] \neq \emptyset. \tag{4.35}$$

We find $N[sq] \subset X_{\nu+2\kappa}(q)$, and hence $\kappa_0 = \nu + 2\kappa + 1$. Consequently we have

$$\kappa_0 = \begin{cases} \nu + 2\kappa + 2 - d & \text{if } t = 1,\ \xi(cq) \neq 1,\ \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \nu + d & \text{if } t = 2,\ c^{-1}q \notin N_{K/F}(\mathfrak{r}), \text{ and } d > 1, \\ \nu + 2\kappa + 1 & \text{if } t = 3,\ \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}, \\ \nu + 1 & \text{otherwise.} \end{cases}$$

This completes the determination of the number κ_0.

4.7. Now, in (4.28) we have $\varphi(k_{i,b}, L) = 2^{-1}\mathfrak{p}^i + \varphi(b, N) + 2^{-1}(q - \varphi[b])\mathfrak{p}^{-i}$ by (2.5), (2.6), and (2.7) for $0 \leq i \leq \kappa_0 - 1$ and $b \in X_i(q)$. Let $m(i, b) \in \mathbf{Z}$ such that $\varphi(k_{i,b}, L) = 2^{-1}\mathfrak{p}^{m(i,b)}$. Here [IQD, Theorem 1.3] implies $k_{i,b}C = L[q, 2^{-1}\mathfrak{p}^{m(i,b)}]$. We have $0 \leq m(i, b) \leq \mu(q - \varphi[b]) - i \leq (\kappa_0 - 1) - i$ in the notation of (3.3), with μ of (4.18). From this and $m(i, b) \leq i$, we see that

$$0 \leq m(i, b) \leq [(\kappa_0 - 1)/2] \tag{4.36}$$

for $0 \leq i \leq \kappa_0 - 1$ and $b \in X_i(q)$. On the other hand, when $\kappa_0 = \nu + 1$, put $z = 0$; when $\kappa_0 > \nu + 1$, take any element $z \in N[sq]$ and fix it. Here s is of (4.30), (4.32), or (4.34) according as $t = 1$, 2, or 3. Then $z \in X_{\kappa_0 - 1}(q)$. We assert that

$$m(i, z) = i \tag{4.37}$$

for $0 \leq i \leq [(\kappa_0 - 1)/2]$. Indeed, if $z = 0$, then it is obvious. Suppose $z \in N[sq]$. Then $\mu(q - \varphi[z]) = \kappa_0 - 1$. From the theorem in the case $r = 0$ and $t > 0$, we find that

$$\varphi(z, N) = \begin{cases} \mathfrak{p}^{(\nu+\delta)/2} & \text{if } t = 1, 3, \\ 2^{-1}\mathfrak{p}^{[(\nu+d)/2]} & \text{if } t = 2. \end{cases}$$

Therefore

$$m(i, z) = \begin{cases} \min(i, \kappa + (\nu + \delta)/2, (\kappa_0 - 1) - i) & \text{if } t = 1, 3, \\ \min(i, [(\nu + d)/2], (\kappa_0 - 1) - i) & \text{if } t = 2. \end{cases}$$

From this, we obtain (4.37). As a consequence, from (4.36) and (4.37),

$$L[q] = \bigcup_{i=0}^{\kappa_0 - 1} \bigcup_{b \in X_i(q)/\mathfrak{p}^i N} k_{i,b}C = \bigsqcup_{i=0}^{[(\kappa_0 - 1)/2]} L[q, 2^{-1}\mathfrak{p}^i]$$

and $L[q, 2^{-1}\mathfrak{p}^i] = k_{i,z}C$. This completes the proof.

5 The maximality of $L \cap (Fh)^{\perp}$

In this section still the field F is local and we prove the second main Theorem 5.3 as an application of Theorem 3.5. We first prepare two lemmas.

5.1 Lemma. *Let ξ be as in Notation. Let $\alpha \in F^{\times}$ such that $\xi(\alpha) \neq 1$. Let $\mathfrak{o}$ be the valuation ring of $F(\sqrt{\alpha})$, $\mathfrak{q}_{\mathfrak{o}}$ the maximal ideal of $\mathfrak{o}$, $\mathfrak{d}_{F(\sqrt{\alpha})/F}$ the different of $F(\sqrt{\alpha})$ relative to F, and μ the normalized order function of F. Then we obtain the following assertions:*

(1) *If $2 \in \mathfrak{g}^{\times}$ and $\mu(\alpha) \in 2\mathbf{Z}$, then $\mathfrak{d}_{F(\sqrt{\alpha})/F} = \mathfrak{o}$.*
(2) *If $\mu(\alpha) \notin 2\mathbf{Z}$, then $\mathfrak{d}_{F(\sqrt{\alpha})/F} = 2\mathfrak{q}_{\mathfrak{o}}$.*
(3) *If $2 \in \mathfrak{p}$, $\mu(\alpha) \in 2\mathbf{Z}$, $\xi(\alpha) = 0$, and $\mathfrak{d}_{F(\sqrt{\alpha})/F} = \mathfrak{q}_{\mathfrak{o}}^{d}$, then $d \in 2\mathbf{Z}$.*

Proof. The first two assertions are well known. Assertion (3) follows from Lemma 4.2(1), (2). □

5.2 Lemma. *Let H be an integral lattice in V. Let t be the core dimension of V. Let $\delta(\varphi)$ be defined as in* (2.1). *Assume $n \notin 2\mathbf{Z}$ and $\delta(\varphi) \cap \mathfrak{g}^{\times} = \emptyset$. Then we have H is maximal in V if and only if $[\tilde{H} : H] = [\mathfrak{g} : 2\mathfrak{p}]$. Here $\tilde{H}$ is defined as in* (2.2).

Proof. Assume that H is maximal in V. Then [AQC, Lemma 6.9] implies $[\tilde{H} : H] = [\tilde{L} : L]$ with L of (2.4). Since $\tilde{L} = \tilde{N} + \sum_{i=1}^{r}(\mathfrak{g}f_i + \mathfrak{g}e_i)$, we have $[\tilde{L} : L] = [\tilde{N} : N]$. By (2.8), (2.11), (2.19), and (2.20), we obtain $[\tilde{N} : N] = [\mathfrak{g} : 2\mathfrak{p}]$ since $\delta = 1$. Thus we obtain the "only if"-part of the assertion. Conversely, we assume that H is an integral lattice in V such that

$$[\tilde{H} : H] = [\mathfrak{g} : 2\mathfrak{p}]. \tag{5.1}$$

By [AQC, Lemma 6.2(1)], there exists a maximal lattice H_0 in V such that $H \subset H_0$. Then

$$H \subset H_0 \subset \tilde{H_0} \subset \tilde{H}. \tag{5.2}$$

From the "only if"-part of the lemma, which is settled above, we obtain $[\tilde{H_0} : H_0] = [\mathfrak{g} : 2\mathfrak{p}]$. Combining this with (5.1) and (5.2), we obtain $H = H_0$, and hence H is maximal in V. □

We remark that the index $[\tilde{H} : H]$ of a maximal lattice H in V is given in [AQC, Lemma 8.4(iv)] when $n \in 2\mathbf{Z}$ or $\delta(\varphi) \cap \mathfrak{g}^{\times} \neq \emptyset$.
Now, for $h \in L$ such that $\varphi[h] \neq 0$, put

$$(Fh)^{\perp} = \{x \in V \mid \varphi(x, h) = 0\}. \tag{5.3}$$

5.3 Theorem. *Let L be a maximal lattice in V and $\tau(q)$ as in* (3.8) *for a given $q \in \mathfrak{g} \cap F^{\times}$. Assume $n \geq 2$. Then for $h \in L$ such that $\varphi[h] \neq 0$, we have*

$$L \cap (Fh)^{\perp} \textit{ is maximal in } (Fh)^{\perp} \Longleftrightarrow h \in L\big[\varphi[h], 2^{-1}\mathfrak{p}^{\tau(\varphi[h])}\big].$$

Hereafter we prove this theorem until the end of §5.14.

5.4. Before stating the proof let us recall the basic notion and terminology in the previous subsections, which will be needed in the next arguments. Put $q = \varphi[h]$, then $h \in L[q]$. Put simply $\tau = \tau(q)$. We have

$$L[q] = \begin{cases} L[q, 2^{-1}\mathfrak{p}^{\tau}] & \text{if } r = 0, \\ \bigsqcup_{i=0}^{\tau} L[q, 2^{-1}\mathfrak{p}^{i}] & \text{if } r \geq 1 \end{cases} \tag{5.4}$$

by (3.8). Hence $h \in L[q, 2^{-1}\mathfrak{p}^i]$ for some $0 \leq i \leq \tau$. Put $W = (Fh)^{\perp}$. Our aim is to show that $L \cap W$ is maximal in W if and only if $i = \tau$.
We have a Witt decomposition of V with respect to φ

$$V = Z + \sum_{j=1}^{r}(Ff_j + Fe_j), \quad L = N + \sum_{j=1}^{r}(\mathfrak{g}f_j + \mathfrak{g}e_j) \tag{5.5}$$

as in (2.4). Let t be the core dimension of (V, φ). Let ξ be as in Notation.
Assume $t = 1$. Let c and δ be as in (2.9) and (2.10), respectively. For q, let d and s be as in Theorem 3.5(ii).
Assume $t = 2$. Let b and c be as in (2.12) and δ as in (2.13). Let K and $\mathfrak{r}$ be as in §2.3(II). Let $\mathfrak{q}$ be the maximal ideal of $\mathfrak{r}$ and $\rho \in Gal(K/F)$ such that $\rho \neq 1$. Let $\mathfrak{d}$ and d be as in Theorem 3.5(iii). Then

$$K \text{ is isomorphic to } F(\sqrt{-bc}), \tag{5.6}$$

$$\mathfrak{d} = \mathfrak{d}_{K/F} = \mathfrak{q}^d \text{ when } \mathfrak{d} \neq \mathfrak{r}. \tag{5.7}$$

For q, let s be as in Theorem 3.5(iii).
Assume $t = 3$. Let c and δ be as in (2.14) and (2.15), respectively. For q, let s be as in Theorem 3.5(iv).
Let $\delta(\varphi)$ be as in (2.1). We may assume that: if $t = 1$ or 3 and $\delta(\varphi) \cap \mathfrak{g}^{\times} \neq \emptyset$, then $c \in \mathfrak{g}^{\times}$; if $t = 1$ or 3 and $\delta(\varphi) \cap \mathfrak{g}^{\times} = \emptyset$, then $c\mathfrak{g} = \mathfrak{p}$; if $t = 2$, then $b, c \in \mathfrak{g}^{\times} \sqcup \pi\mathfrak{g}^{\times}$; if $t = 2$ and K is ramified over F, then $c \in \mathfrak{g}^{\times}$; see §2.3.

5.5. First suppose that:

$t = 1$, $r \geq 1$, and $\xi(cq) = 1$; or
$t = 2$ and $c^{-1}q \in N_{K/F}(\mathfrak{r})$; or
$t = 3$ and $\xi(-cq) \neq 1$; or
$t = 4$.

This assumption is equivalent to $N[q] \neq \emptyset$ by Lemma 3.4. Here $0 \neq q = \varphi[h]$, $h \in L$. Then $h \in L[q, 2^{-1}\mathfrak{p}^i]$ for some $0 \leq i \leq \tau$ by (5.4). We obtain

$$L[q, 2^{-1}\mathfrak{p}^i] = \begin{cases} yC & \text{if } i = \tau, \\ h_{i,y}C & \text{if } i < \tau \end{cases} \tag{5.8}$$

by (3.13), (3.16), (3.19), and (3.21). Here, y is any element of $N[q]$ and fix it.

We first prove that $L \cap W$ is maximal in W when $i = \tau$. In this case, $h \in L[q, 2^{-1}\mathfrak{p}^\tau] = yC$ by (5.8). Therefore there exists $\gamma \in C$ such that $y = h\gamma$. We have $L \cap (Fy)^\perp = (L \cap W)\gamma$ since $L\gamma = L$ and $(Fy)^\perp = W\gamma$. Therefore $L \cap (Fy)^\perp$ is maximal in $(Fy)^\perp$ if and only if $L \cap W$ is maximal in W. Hence we assume $h = y$ and $W = (Fy)^\perp$. Now, we have

$$W = (Z \cap W) + \sum_{j=1}^{r} (Ff_j + Fe_j)$$

since $h \in N$, (5.3), and (5.5). This is a Witt decomposition of W with respect to the restriction of φ to W. Moreover we obtain

$$(5.9)\quad L \cap W = (N \cap W) + \sum_{j=1}^{r} (\mathfrak{g}f_j + \mathfrak{g}e_j), \quad N \cap W = \{x \in Z \cap W \mid \varphi[x] \in \mathfrak{g}\}$$

from (2.7) and (5.5). Thus by [AQC, Lemma 6.5], $L \cap W$ is maximal in W when $i = \tau$.

Next suppose $i < \tau$. We shall show that $L \cap W$ is not a maximal lattice in W in this case. We obtain $h \in h_{i,y}C$ by (5.8). Thus we may assume $h = h_{i,y}$. By (3.8), $N[q] = N[q, 2^{-1}\mathfrak{p}^\tau]$. From this,

$$(5.10)\qquad \varphi(y, N) = 2^{-1}\mathfrak{p}^\tau.$$

We see that

(5.11)

$$W = X + \sum_{j=1}^{r-1} (Ff_j + Fe_j), X = \{ae_r + x - 2\pi^{-i}\varphi(y, x)f_r \mid a \in F, x \in Z\},$$

$$L \cap W = H + \sum_{j=1}^{r-1} (\mathfrak{g}f_j + \mathfrak{g}e_j), H = \{ae_r + x - 2\pi^{-i}\varphi(y, x)f_r \mid a \in \mathfrak{g}, x \in N\}$$

by the definition of $h_{i,y}$ (in (3.7)), (5.3), (5.5), and (5.10). Take

$$(5.12)\qquad w \in N \text{ such that } \varphi(y, w) = -2^{-1}\pi^\tau$$

and fix it. Put $u = \pi^{\tau - i}f_r + w - \pi^{i-\tau}\varphi[w]e_r$, $v = \pi^{i-\tau}e_r$, and

$$Y = \{x - 2\pi^{i-\tau}\varphi(x, w)e_r \mid x \in Z \text{ such that } \varphi(x, y) = 0\}.$$

Then we find that $X = Y + Fu + Fv$ is a Witt decomposition of X by a straightforward calculation. Here X is defined as in (5.11). Put $\Lambda = \{k \in Y \mid \varphi[k] \in \mathfrak{g}\}$, then $\Lambda + \mathfrak{g}u + \mathfrak{g}v$ is maximal in X by [AQC, Lemma 6.5]. We assert that $H \subsetneq \Lambda + \mathfrak{g}u + \mathfrak{g}v$. Indeed, it is clear that $v \notin H$ since $i - \tau < 0$. For any $\ell = ae_r + x - 2\pi^{-i}\varphi(y, x)f_r \in H$, put $\xi = -2\pi^{-\tau}\varphi(y, x)$ and $\eta = a\pi^{\tau - i} + 2\pi^{-\tau}\varphi(y, x)\varphi[w] + 2\varphi(x, w)$ with w in (5.12). Then a straightforward computation shows that $\xi, \eta \in \mathfrak{g}$ and $\ell - \xi u - \eta v \in \Lambda$ by (5.10). Therefore $H \subsetneq \Lambda + \mathfrak{g}u + \mathfrak{g}v$. Thus H is not maximal in X, and hence $L \cap W$ is not maximal in W by [AQC, Lemma 6.3]. This completes the proof in the case $N[q] \neq \emptyset$.

5.6. Let us now suppose that:

$t = 0$ and $r \geq 1$; or
$t = 1$, $r \geq 1$, $\xi(cq) \neq 1$, and $2 \in \mathfrak{g}^\times$; or
$t = 1$, $r \geq 1$, $\xi(cq) \neq 1$, and $\nu \not\equiv \delta \pmod 2$; or
$t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, and $\mathfrak{d}_{K/F} = \mathfrak{r}$; or
$t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, and $\mathfrak{d}_{K/F} = \mathfrak{q}$; or
$t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{g}^\times$.

Here $\nu \in \mathbf{Z}$ such that $q\mathfrak{g} = \mathfrak{p}^\nu$ with $0 \neq q = \varphi[h]$, $h \in L$. In this case we obtain

$$L[q] = \begin{cases} \sqcup_{j=0}^{\tau} \ell_j C & \text{if } t \geq 1 \text{ or } r \geq 2, \\ \sqcup_{j=0}^{\nu} \ell_j C & \text{if } t = 0 \text{ and } r = 1 \end{cases}$$

with ℓ_j in (3.7) and $\tau = [\nu/2]$ of Theorem 3.5. Moreover

$$N[q] = \emptyset \tag{5.13}$$

by Lemma 3.4. We have $h \in L[q, 2^{-1}\mathfrak{p}^i]$ for some $0 \leq i \leq \tau$ by (5.4). Hereafter until the end of §5.7 we prove the theorem in the case $t \geq 1$ or $r \geq 2$. Then

$$L[q, 2^{-1}\mathfrak{p}^i] = \ell_i C \text{ for } 0 \leq i \leq \tau$$

by (3.10), (3.13), (3.16), and (3.19). Thus we may assume $h = \ell_i$ and $W = (F\ell_i)^\perp$ since $h \in \ell_i C$.
In this §5.6 we determine $[(L \cap W)\tilde{} : L \cap W]$. Put

$$w = f_r - q\pi^{-2i} e_r \tag{5.14}$$

with e_r and f_r in (5.5). Then

$$W = (Fw + Z) + \sum_{j=1}^{r-1} (Ff_j + Fe_j) \tag{5.15}$$

from the definition of ℓ_i (in (3.7)), (5.3), and (5.5). We understand that: $\sum_{j=1}^{r-1}(Ff_j + Fe_j) = \{0\}$ when $t > 0$ and $r = 1$; $Z = \{0\}$ when $t = 0$ and $r \geq 2$. We assert that (5.15) is a Witt decomposition. Indeed, it is clear when $t = 0$ and $r \geq 2$. Assume $t \geq 1$. If $\varphi[aw + x] = 0$ for $a \in F$ and $x \in Z$, then $\varphi[x] = q\pi^{-2i}a^2$. If $a \neq 0$, then this is the case if and only if $\varphi[a^{-1}\pi^i x] = q$, and hence $N[q] \neq \emptyset$. This contradicts (5.13). Thus $a = 0$, and hence $x = 0$. Therefore the restriction of φ to $Fw + Z$ is anisotropic. Combining this with

(2.5), (2.6), and (5.14), we see that (5.15) is a Witt decomposition. Now, we have

$$L \cap W = (\mathfrak{g}w + N) + \sum_{j=1}^{r-1} (\mathfrak{g}f_j + \mathfrak{g}e_j) \tag{5.16}$$

by (5.5) and (5.15). Therefore a straightforward computation shows that

$$(L \cap W)\tilde{} = 2^{-1}\mathfrak{p}^{2i-\nu}w + \tilde{N} + \sum_{j=1}^{r-1} (\mathfrak{g}f_j + \mathfrak{g}e_j) \tag{5.17}$$

from (2.2) with (5.16). Combining (5.16) with (5.17), we have

$$[(L \cap W)\tilde{} : L \cap W] = [\mathfrak{g} : 2\mathfrak{p}^{\nu-2i}] \cdot [\tilde{N} : N]. \tag{5.18}$$

Here we obtain the index $[\tilde{N} : N]$ by [AQC, Lemma 8.4(iv)] and Lemma 5.2. Combining this with (5.18), we have

(5.19)

$$[(L \cap W)\tilde{} : L \cap W] = \begin{cases} [\mathfrak{g} : 2\mathfrak{p}^{\nu-2i}] & \text{if } t = 0 \text{ and } r \geq 2, \\ [\mathfrak{g} : 4\mathfrak{p}^{\nu-2i+\delta}] & \text{if } t = 1, r \geq 1, \xi(cq) \neq 1, \text{ and } 2 \in \mathfrak{g}^{\times}, \\ [\mathfrak{g} : 4\mathfrak{p}^{\nu-2i+\delta}] & \text{if } t = 1, r \geq 1, \xi(cq) \neq 1, \text{ and } \nu \not\equiv \delta \pmod 2, \\ [\mathfrak{g} : 2\mathfrak{p}^{\nu-2i+2\delta}] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), \text{ and } \mathfrak{d} = \mathfrak{r}, \\ [\mathfrak{g} : 2\mathfrak{p}^{\nu-2i+1}] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), \text{ and } \mathfrak{d} = \mathfrak{q}, \\ [\mathfrak{g} : \mathfrak{p}^{\nu-2i+2-\delta}] & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{g}^{\times}. \end{cases}$$

Note that: if $t = 2$, $r \geq 1$, and $\mathfrak{d} = \mathfrak{r}$, then $c^{-1}q \notin N_{K/F}(\mathfrak{r})$ if and only if $\nu \not\equiv \delta \pmod 2$ by Lemma 3.4(2); if $t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{g}^{\times}$, then $\nu \equiv \delta \pmod 2$.

5.7. In this § we still assume $t \geq 1$ or $r \geq 2$. For an integral lattice R in W, the following assertion holds:

(5.20)

R is maximal in W

$$\Longleftrightarrow [\tilde{R}:R] = \begin{cases} [\mathfrak{g}:2\mathfrak{p}^{\nu-2\tau}] & \text{if } t=0 \text{ and } r\geq 2,\\ [\mathfrak{g}:\mathfrak{p}^{2\delta}] & \text{if } t=1, r\geq 1, \xi(cq)\neq 1,\\ & \quad\text{and } \nu\equiv\delta \pmod 2,\\ [\mathfrak{g}:4\mathfrak{p}] & \text{if } t=1, r\geq 1, \xi(cq)\neq 1,\\ & \quad\text{and } \nu\not\equiv\delta \pmod 2,\\ [\mathfrak{g}:2\mathfrak{p}^{1+\delta}] & \text{if } t=2, r\geq 1, c^{-1}q\notin N_{K/F}(\mathfrak{r}), \text{ and } \mathfrak{d}=\mathfrak{r},\\ [\mathfrak{g}:2\mathfrak{p}^{\nu-2\tau+1}] & \text{if } t=2, r\geq 1, c^{-1}q\notin N_{K/F}(\mathfrak{r}), \text{ and } \mathfrak{d}=\mathfrak{q},\\ [\mathfrak{g}:\mathfrak{p}^{2}] & \text{if } t=3, r\geq 1, \xi(-cq)=1, \text{ and } 2\in\mathfrak{g}^{\times}. \end{cases}$$

Note that if $t=1$, $r\geq 1$, $\xi(cq)\neq 1$, and $\nu\equiv\delta \pmod 2$, then $2\in\mathfrak{g}^{\times}$. If (5.20) holds, then combining (5.19) with (5.20), we obtain our theorem in the case $t\geq 1$ or $r\geq 2$ since $L\cap W$ is an integral lattice in W. Let us prove (5.20). We observe a core subspace $Fw+Z$ of W with w of (5.14). If $t=0$ and $r\geq 2$, then $\dim_F(Fw+Z)=1$ and $\delta(Fw+Z,\varphi)=\varphi[w]F^{\times 2}=-qF^{\times 2}$. Here $\delta(Fw+Z,\varphi)$ is defined as in (2.1). This implies $\delta(Fw+Z,\varphi)\cap\mathfrak{g}^{\times}\neq\emptyset$ if $\nu\in 2\mathbf{Z}$ and $\delta(Fw+Z,\varphi)\cap\mathfrak{g}^{\times}=\emptyset$ if $\nu\notin 2\mathbf{Z}$. Therefore we have (5.20) by [AQC, Lemma 8.4(iv)] and Lemma 5.2 when $t=0$ and $r\geq 2$. Assume $t=1$, $r\geq 1$, and $\xi(cq)\neq 1$. Since $\varphi[w]=-q\pi^{-2i}$ and $Z=Fg$ with g of (2.8), $(Fw+Z,\varphi)$ is isomorphic to $(F(\sqrt{cq}),\psi)$, where $\psi[x]=cN_{F(\sqrt{cq})/F}(x)$ for $x\in F(\sqrt{cq})$, as explained in §2.3(II). Suppose $\nu\equiv\delta \pmod 2$, then $2\in\mathfrak{g}^{\times}$. Thus Lemma 5.1(1) implies that $F(\sqrt{cq})$ is unramified. Therefore we have (5.20) in this case by [AQC, Lemma 8.4(iv)]. Next suppose $\nu\not\equiv\delta \pmod 2$, then $\mathfrak{d}_{F(\sqrt{cq})/F}=2\mathfrak{q}_{F(\sqrt{cq})}$ by Lemma 5.1(2), where $\mathfrak{q}_{F(\sqrt{cq})}$ is the maximal ideal of the valuation ring of $F(\sqrt{cq})$. Therefore [AQC, Lemma 8.4(iv)] implies (5.20) when $t=1$, $r\geq 1$, $\xi(cq)\neq 1$, and $2\in\mathfrak{g}^{\times}$ or $\nu\not\equiv\delta \pmod 2$. Assume $t=2$, $r\geq 1$, and $c^{-1}q\notin N_{K/F}(\mathfrak{r})$, then $\dim_F(Fw+Z)=3$. Since $Z=Fg_1+Fg_2$ with g_1 and g_2 in (2.12) and $\varphi[w]=-q\pi^{-2i}$, we have

$$\delta(Fw+Z,\varphi)=bcqF^{\times 2}. \tag{5.21}$$

Suppose $\mathfrak{d}=\mathfrak{r}$. Then $\nu\not\equiv\delta \pmod 2$ by Lemma 3.4(2). Since K is unramified over F, we have $b\mathfrak{g}=c\mathfrak{g}(=\mathfrak{p}^{\delta})$ by Lemma 5.1(2). Thus (5.21) implies $\delta(Fw+Z,\varphi)\cap\mathfrak{g}^{\times}=\emptyset$ if $\delta=0$ and $\delta(Fw+Z,\varphi)\cap\mathfrak{g}^{\times}\neq\emptyset$ if $\delta=1$. From this we obtain (5.20) by [AQC, Lemma 8.4(iv)] and Lemma 5.2 in this case. Next suppose $\mathfrak{d}=\mathfrak{q}$. Here Lemma 5.1 implies $b\mathfrak{g}=\mathfrak{p}$ since $c\in\mathfrak{g}^{\times}$. Therefore (5.21) implies $\delta(Fw+Z,\varphi)\cap\mathfrak{g}^{\times}=\emptyset$ if $\nu\in 2\mathbf{Z}$ and $\delta(Fw+Z,\varphi)\cap\mathfrak{g}^{\times}\neq\emptyset$ if $\nu\notin 2\mathbf{Z}$. Hence we have (5.20) by [AQC, Lemma 8.4(iv)] and Lemma 5.2 when $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, and $\mathfrak{d}_{K/F} = \mathfrak{r}$ or $\mathfrak{q}$. Finally if $t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{g}^\times$, then $\dim_F(Fw + Z) = 4$, and hence [AQC, Lemma 8.4(iv)] implies (5.20). This proves the theorem in the case when $N[q] = \emptyset$, $L[q] = \sqcup_j \ell_j C$, and $t \geq 1$ or $r \geq 2$.

5.8. In this § we prove the theorem in the case $t = 0$ and $r = 1$. Then

$$L[q, 2^{-1}\mathfrak{p}^i] = \begin{cases} \ell_i C \sqcup \ell_{\nu-i} C & \text{if } t = 0,\ r = 1,\ \text{and } i \neq \nu/2, \\ \ell_i C & \text{if } t = 0,\ r = 1,\ \text{and } i = \nu/2 \end{cases}$$

for $0 \leq i \leq \tau$, by (3.10). Since $h \in L[q, 2^{-1}\mathfrak{p}^i]$ for some $0 \leq i \leq \tau$ by (5.4), we may assume that $h = \ell_i$ or $h = \ell_{\nu-i}$ when $i \neq \nu/2$ and $h = \ell_i$ when $i = \nu/2$. If $h = \ell_i$ for $0 \leq i \leq \tau$ (including the case $h = \ell_{\nu/2}$), we can obtain the assertion in the same way as §§5.6 and 5.7. Assume $h = \ell_{\nu-i}$ for $0 \leq i < \nu/2$. Put here $w = f_1 - q\pi^{-2(\nu-i)}e_1$. Then we see that

$$W = (F\ell_{\nu-i})^\perp = Fw, \quad L \cap W = \mathfrak{p}^{\nu-2i}w, \text{ and } (L \cap W)^{\sim} = 2^{-1}\mathfrak{g}w$$

in a similar way as §5.6. Thus $[(L \cap W)^{\sim} : L \cap W] = [\mathfrak{g} : 2\mathfrak{p}^{\nu-2i}]$. Therefore we obtain the theorem in the same way as in the case when $t = 0$ and $r \geq 2$ since $\varphi[w]F^{\times 2} = -qF^{\times 2}$. This completes the proof in the case when $N[q] = \emptyset$ and $L[q] = \sqcup_j \ell_j C$.

5.9. Finally we suppose that:

$t = 1$, $r \geq 1$, $\nu \equiv \delta \pmod 2$, $\xi(cq) \neq 1$, and $2 \in \mathfrak{p}$; or
$t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, and $d > 1$; or
$t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{p}$.

Note that $c \in \mathfrak{g}^\times$ when $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, and $d > 1$. Then we have

$$L[q] = \bigsqcup_{j=0}^{\tau} k_{j,z}C \text{ and } k_{j,z}C = L[q, 2^{-1}\mathfrak{p}^j] \tag{5.22}$$

with $k_{j,z}$ in (3.7), from (3.8), (3.13), (3.16), and (3.19). Here z is any element of $N[sq]$ with s of (3.11), (3.14), or (3.17) of Theorem 3.5 according as $t = 1, 2$, or 3. We fix z. We obtain
(5.23)

$$\tau = \begin{cases} \kappa + \left[\frac{\nu+1-d}{2}\right] & \text{if } t = 1, r \geq 1, \xi(cq) \neq 1, \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \left[\frac{\nu+d-1}{2}\right] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), \text{ and } d > 1, \\ \kappa + \left[\frac{\nu}{2}\right] & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p} \end{cases}$$

from (3.12), (3.15), and (3.18), where $\kappa \in \mathbf{Z}$ such that $2\mathfrak{g} = \mathfrak{p}^\kappa$. Moreover, by Lemma 3.4,

$$N[q] = \emptyset. \tag{5.24}$$

Applying Theorem 3.5 to (Z,φ), N, and sq, we have $N[sq] = N[sq, 2^{-1}\mathfrak{p}^{\tau(sq)}]$ by (3.8). Here

$$(5.25)\tau(sq) = \begin{cases} \kappa + \frac{\nu+\delta}{2} & \text{if } t = 1, r \geq 1, \xi(cq) \neq 1, \\ & \quad \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \left[\frac{\nu+d}{2}\right] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), \text{ and } d > 1, \\ \kappa + \frac{\nu+\delta}{2} & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p} \end{cases}$$

from (3.12), (3.15), and (3.18). Thus

$$\varphi(z, N) = 2^{-1}\mathfrak{p}^{\tau(sq)}. \tag{5.26}$$

Assume $h \in L[q, 2^{-1}\mathfrak{p}^i]$ for some $0 \leq i \leq \tau$. Then by (5.22), $h \in k_{i,z}C$, and hence we may assume $h = k_{i,z}$. Hereafter we show that $L \cap W$ is maximal in W if and only if $i = \tau$. Put

$$x_1 = \pi^{i-\tau}[f_r - \pi^{-2i}(q - \varphi[z])e_r] \tag{5.27}$$

with e_r and f_r in (5.5). Then

$$\varphi[x_1] = \pi^{-2\tau}(s-1)q \text{ and } \pi^{\tau-i}x_1 \in L. \tag{5.28}$$

By a straightforward computation, we obtain
(5.29)

$$W = X + \sum_{j=1}^{r-1}(Ff_j + Fe_j), \quad X = \{ax_1 + x - 2\pi^{-i}\varphi(x,z)e_r \mid a \in F, x \in Z\}$$

with x_1 of (5.27). Then (5.29) is a Witt decomposition. Indeed, if $\varphi[ax_1 + x - 2\pi^{-i}\varphi(x,z)e_r] = 0$ for $a \in F$ and $x \in Z$, then $\varphi[x - \pi^{-\tau}az] = (\pi^{-\tau}a)^2q$. Assuming $a \neq 0$, we have $\varphi[\pi^{\tau}a^{-1}x - z] = q$, and hence $N[q] \neq \emptyset$. This contradicts (5.24). Thus $a = 0$, and hence $x = 0$. Therefore the restriction of φ to X is anisotropic. Combining this with (2.5), (2.6), and (5.27), we see that (5.29) is a Witt decomposition. Now, we easily see that $2\pi^{-i}\varphi(x,z) \in \mathfrak{g}$ for $x \in N$ from (5.23), (5.25), (5.26), and $0 \leq i \leq \tau$. From this and (5.28),
(5.30)

$$L \cap W = H + \sum_{j=1}^{r-1}(\mathfrak{g}f_j + \mathfrak{g}e_j), \quad H = \{ax_1 + x - 2\pi^{-i}\varphi(x,z)e_r \mid a \in \mathfrak{p}^{\tau-i}, x \in N\}.$$

By [AQC, Lemma 6.3(1)], $L \cap W$ is maximal in W if and only if H is maximal in X. Thus we consider the lattice H in X instead of $L \cap W$ in W.

5.10. In this § we first determine the structure of N under the assumption of §5.9. Now we put

$$Y = \{k \in Z \mid \varphi(k,z) = 0\} \text{ and } z_1 = \pi^{-[\nu/2]}z. \tag{5.31}$$

Then $Z = Fz_1 + Y$.
First assume $t = 1$, $r \geq 1$, $\nu \equiv \delta \pmod 2$, $\xi(cq) \neq 1$, and $2 \in \mathfrak{p}$. Since $\varphi[z_1]\mathfrak{g} = \mathfrak{p}^\delta$,

$$N = \mathfrak{g}z_1. \tag{5.32}$$

Next assume $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, and $d > 1$. Then Lemma 5.1(1) and (2) imply $2 \in \mathfrak{p}$. Take $y \in Y$ such that $Y = Fy$, then

$$Z = Fz_1 + Fy. \tag{5.33}$$

Thus from (2.1) and (2.12), we have $\varphi[z_1]\varphi[y]F^{\times 2} = -\delta(Z, \varphi) = bcF^{\times 2}$, and hence we may assume

$$\varphi[z_1]\varphi[y](bc)^{-1} = \begin{cases} 1 & \text{if } b\mathfrak{g} = \mathfrak{p}, \\ \pi^{2\lambda} & \text{if } b \in \mathfrak{g}^\times, \end{cases} \tag{5.34}$$

where

$$\lambda = \nu - 2[\nu/2]. \tag{5.35}$$

From (5.6) and (5.34), we see that $F + Fz_1y \subset A(Z, \varphi)$ is isomorphic to K. Here we identify $F + Fz_1y$ with K. Suppose $b\mathfrak{g} = \mathfrak{p}$. Then

$$d = 2\kappa + 1 \tag{5.36}$$

by $c \in \mathfrak{g}^\times$, Lemma 5.1(2), and (5.7). Put

$$z_\nu = \begin{cases} z_1 & \text{if } \nu \in 2\mathbf{Z}, \\ y & \text{if } \nu \notin 2\mathbf{Z}. \end{cases}$$

Then $\varphi[z_\nu] \in \mathfrak{g}^\times$ from (5.31) and (5.34), and hence $Z = Kz_\nu$ and $N = \mathfrak{r}z_\nu$ by (5.33). We find $z_1y \in \mathfrak{r}$ and $(z_1y - (z_1y)^\rho)\mathfrak{r} = 2\mathfrak{q} = \mathfrak{d}$, and hence $\mathfrak{r} = \mathfrak{g}[z_1y]$ by [AQC, Lemma 5.6(ii)]. Thus

$$N = \mathfrak{g}z_1 + \mathfrak{g}y. \tag{5.37}$$

Next suppose $b \in \mathfrak{g}^\times$. Then $bc \in \mathfrak{g}^\times$ and $2 \in \mathfrak{p}$ from $c \in \mathfrak{g}^\times$, $d > 1$, and Lemma 5.1(1). Thus there exist

$$\alpha, \beta \in \mathfrak{g}^\times \text{ such that } -bc = \alpha^{-2}(1 + \pi^{2\kappa+1-d}\beta) \tag{5.38}$$

by $d > 1$ and Lemma 4.2(1). Put $\eta = \pi^{(d-2\kappa)/2}(1 + \alpha\pi^{-\lambda}z_1y)$ in K with λ of (5.35). Then η is a root of an Eisenstein equation $\mathbf{x}^2 - 2\pi^{(d-2\kappa)/2}\mathbf{x} - \pi\beta = 0$, and hence η is a prime element of K and $(\eta - \eta^\rho)\mathfrak{r} = (2\eta - 2\pi^{(d-2\kappa)/2})\mathfrak{r} = \mathfrak{d}$. Here $\mathbf{x}$ is an indeterminate. Thus $\mathfrak{r} = \mathfrak{g}[\eta]$ by [AQC, Lemma 5.6(ii)]. By (5.31) and (5.34), we have $\varphi[y]\mathfrak{g} = \mathfrak{p}^{\lambda}$. From this and $\eta^{-1} = -\pi^{-1+(d-2\kappa)/2}\beta^{-1}(1 - \alpha\pi^{-\lambda}z_1y)$, we obtain

$$N = \mathfrak{r}\eta^{-\lambda}y = \mathfrak{g}y + \mathfrak{g}\pi^{-\lambda+(d-2\kappa)/2}[y + (-1)^{\nu}\alpha\pi^{-\lambda}\varphi[y]z_1]. \tag{5.39}$$

Finally assume $t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{p}$. Then $\nu \equiv \delta \pmod 2$, and hence $\varphi[z_1]\mathfrak{g} = \mathfrak{p}^{\delta}$. We can take

$$y_1, y_2 \in Y \text{ so that } Y = Fy_1 + Fy_2 \text{ and } \varphi(y_1, y_2) = 0 \tag{5.40}$$

by [EPE, Lemma 1.8]. Then we may assume

$$\varphi[y_1]\varphi[y_2] \in \mathfrak{g}^{\times} \tag{5.41}$$

since

$$-\varphi[z_1]\varphi[y_1]\varphi[y_2]F^{\times 2} = \delta(Z, \varphi) = -cF^{\times 2} \tag{5.42}$$

by (2.14), (5.31), and (5.40). Put

$$T = Fy_1y_2 + Fz_1y_1 + Fz_1y_2,\ K_Y = F + Fy_1y_2,\ B = F + T,\ \zeta = z_1y_1y_2 \tag{5.43}$$

in $A(Z)$. Moreover put $c_1 = \varphi[z_1]\varphi[y_1]\varphi[y_2]$. Then $Z = T\zeta$, $Y = K_Yy_2$, B is a division quaternion algebra over F, $c_1\mathfrak{g} = c\mathfrak{g}$, and $\varphi[x\zeta] = c_1N_{B/F}(x)$ for $x \in T$. From $\xi(-cq) = 1$ and (5.42), we have $(y_1y_2)^2F^{\times 2} = sF^{\times 2}$. Thus K_Y is an unramified quadratic extension of F by (3.17). We may assume

$$\varphi[y_1]\mathfrak{g} = \varphi[y_2]\mathfrak{g} = \mathfrak{g} \text{ or } \varphi[y_1]^{-1}\mathfrak{g} = \varphi[y_2]\mathfrak{g} = \mathfrak{p} \tag{5.44}$$

by (5.41). Then we see that

$$\varphi[y_2]\mathfrak{g} = \mathfrak{p}^{1-\delta} = \begin{cases} \mathfrak{p} & \text{if } \nu \equiv 0 \pmod 2, \\ \mathfrak{g} & \text{if } \nu \equiv 1 \pmod 2 \end{cases} \tag{5.45}$$

as shown below. Put

$$\omega = z_1y_1 \text{ and } v = y_1y_2.$$

Then $B = K_Y + K_Y\omega$, $\omega v = -v\omega$, $\omega^2\mathfrak{g} = \mathfrak{p}^{2\delta-1}$, $v \in K_Y \cap T$, and $v^2 \in \mathfrak{g}^{\times}$ from (5.31), (5.40), (5.41), (5.42), (5.43), and (5.45). Therefore

$$N = (\mathfrak{g}v + \mathfrak{r}_Y\omega^{-1})\zeta = \mathfrak{g}z_1 + \mathfrak{r}_Yy_2; \tag{5.46}$$

see §2.3. Here $\mathfrak{r}_Y$ is the valuation ring of K_Y. Now we assert (5.45). Indeed, if this is not the case, then

$$\varphi[y_2]\mathfrak{g} = \mathfrak{p}^{\delta} = \begin{cases} \mathfrak{g} & \text{if } \nu \equiv 0 \pmod 2, \\ \mathfrak{p} & \text{if } \nu \equiv 1 \pmod 2 \end{cases}$$

by (5.44). Since K_Y is unramified over F, there exists $\theta \in B$ such that $B = K_Y + K_Y\theta$, $\theta^2\mathfrak{g} = \mathfrak{p}$, and $\theta y_1 y_2 = -y_1 y_2 \theta$ by the proof of [AQC, Theorem 5.13]. Then we easily see that $\theta \in Fz_1y_1 + Fz_1y_2$. Put $J = Fz_1y_1 + Fz_1y_2$ and $\psi[x] = N_{B/F}(x)$ for $x \in J$. We consider the Clifford algebra $A(J,\psi)$ of ψ. Put $K_J = F + Fz_1y_1 \cdot z_1y_2$, then $J = K_J z_1 y_2$, $\psi[z_1y_2]\mathfrak{g} = \mathfrak{p}^{2\delta}$, and K_J is isomorphic to $F(\sqrt{s})$ which is an unramified quadratic extension of F. Thus Lemma 3.4(2) implies $\Lambda_J[\psi[\theta]] = \emptyset$, where Λ_J is a maximal lattice in J. Since $\theta^2\mathfrak{g} = \mathfrak{p}$, this gives a contradiction, and hence $\varphi[y_2]\mathfrak{g} = \mathfrak{p}^{1-\delta}$.

5.11. Put

$$x_2 = \pi^{-[\nu/2]}(z - 2\pi^{-i}\varphi[z]e_r). \tag{5.47}$$

Then $\varphi[x_2] = \varphi[z_1]$ with z_1 in (5.31). From (5.30), (5.32), (5.37), (5.39), and (5.46),

$$H = \begin{cases} \mathfrak{p}^{\tau-i}x_1 + \mathfrak{g}x_2 & \text{if } t = 1, r \geq 1, \xi(cq) \neq 1, \\ & \quad \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \mathfrak{p}^{\tau-i}x_1 + \mathfrak{g}x_2 + \mathfrak{g}y & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \\ & \quad \text{and } b\mathfrak{g} = \mathfrak{p}, \\ \mathfrak{p}^{\tau-i}x_1 + \mathfrak{g}x_3 + \mathfrak{g}y & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \\ & \quad \text{and } b \in \mathfrak{g}^\times, \\ \mathfrak{p}^{\tau-i}x_1 + \mathfrak{g}x_2 + \mathfrak{r}_Y y_2 & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p} \end{cases} \tag{5.48}$$

with x_1 of (5.27), $y \in Y$ satisfying (5.34), y_2 of (5.40), and $\mathfrak{r}_Y$ in (5.46). Moreover x_3 is given as

$$x_3 = \pi^{-\lambda+(d-2\kappa)/2}[y + (-1)^\nu \alpha \pi^{-\lambda}\varphi[y]x_2], \tag{5.49}$$

with λ of (5.35).

5.12. On the other hand for the space X in (5.29) we put

$$\Lambda = \{x \in X \mid \varphi[x] \in \mathfrak{g}\}. \tag{5.50}$$

Then [AQC, Lemma 6.4] implies that Λ is a unique maximal lattice in X. Here we put

$$w = -\pi^i(q - \varphi[z])^{-1}\varphi[z]f_r + z - \pi^{-i}\varphi[z]e_r \tag{5.51}$$

with e_r and f_r in (5.5). Then we find that

$$x_2 = \pi^{-[\nu/2]}[w + \pi^\tau(q - \varphi[z])^{-1}\varphi[z]x_1], \tag{5.52}$$

$$\varphi[w] = (1-s)^{-1}sq, \tag{5.53}$$

$$X = Fx_1 + Fw + Y,\ \varphi(x_1, w) = 0,\ Y = \{k \in X \mid \varphi(k, x_1) = \varphi(k, w) = 0\}. \tag{5.54}$$

Here Y is given in (5.31) and x_2 is of (5.47).

5.13. In §§5.13 and 5.14 we determine the structure of Λ in the above (5.50). In §5.13 we suppose that: $t = 1$, $r \geq 1$, $\nu \equiv \delta \pmod 2$, $2 \in \mathfrak{p}$, and $\xi(cq) \neq 1$; or $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b\mathfrak{g} = \mathfrak{p}$; or $t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{p}$. (The case when $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b \in \mathfrak{g}^\times$ will be treated in §5.14.) To prove the theorem in this case, it suffices to show that

(5.55)

$$\Lambda = \begin{cases} \mathfrak{g}x_1 + \mathfrak{g}x_2 & \text{if } t = 1, r \geq 1, \xi(cq) \neq 1, \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \mathfrak{g}x_1 + \mathfrak{g}x_2 + \mathfrak{g}y & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \text{ and } b\mathfrak{g} = \mathfrak{p}, \\ \mathfrak{g}x_1 + \mathfrak{g}x_2 + \mathfrak{r}_Y y_2 & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p} \end{cases}$$

by (5.48).
First we shall show that

$$\mathfrak{g}x_1 + \mathfrak{g}x_2 \text{ is maximal in } Fx_1 + Fw. \tag{5.56}$$

For the purpose, we consider the Clifford algebra $A(Fx_1+Fw)$ of the restriction of φ to $Fx_1 + Fw$. Put $E = F + Fwx_1$ in $A(Fx_1 + Fw)$. Then we obtain that

$$Fx_1 + Fw = Ex_1, \ \varphi[xx_1] = \varphi[x_1]N_{E/F}(x) \text{ for } x \in E, \tag{5.57}$$

and E is isomorphic to $F(\sqrt{s})$ since $(wx_1)^2F^{\times 2} = sF^{\times 2}$ by (5.28) and (5.53).
First we suppose that:

$t = 1$, $r \geq 1$, $\xi(cq) = 0$, $\nu \notin 2\mathbf{Z}$, $2 \in \mathfrak{p}$, and $\delta = 1$; or
$t = 1$, $r \geq 1$, $\xi(cq) = -1$, $\nu \equiv \delta \pmod 2$, and $2 \in \mathfrak{p}$; or
$t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b\mathfrak{g} = \mathfrak{p}$; or
$t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{p}$.

Then

$$\mathfrak{D}_{E/F} = \begin{cases} \mathfrak{p}^d & \text{if } t = 1, r \geq 1, \xi(cq) = 0, \nu \notin 2\mathbf{Z}, 2 \in \mathfrak{p}, \text{ and } \delta = 1, \\ \mathfrak{g} & \text{otherwise.} \end{cases} \tag{5.58}$$

Indeed, if $t = 1$, $r \geq 1$, $\xi(cq) = 0$, $\nu \notin 2\mathbf{Z}$, $2 \in \mathfrak{p}$, and $\delta = 1$, then $cqF^{\times 2} = sF^{\times 2}$. Thus we have (5.58) by the definition of d; see Theorem 3.5(ii). If $t = 1$, $r \geq 1$, $\xi(cq) = -1$, $\nu \equiv \delta \pmod 2$, and $2 \in \mathfrak{p}$, then from (3.11), Lemma 4.2(1), and $cq \notin F^{\times 2}$, we have $\varepsilon(s) = 2\kappa$ with ε of (4.11). Thus we obtain (5.58). If $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b\mathfrak{g} = \mathfrak{p}$, then $\varepsilon(s) = 2\kappa$ from (3.14), (5.36), and $c^{-1}q \notin N_{K/F}(\mathfrak{r})$. If $t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{p}$, then clearly we have (5.58) by (4.34) and Lemma 4.2(1). Therefore we have (5.58) for all cases. Now, by (5.23), (5.36), and Lemma 5.1(3),

$$\tau = \begin{cases} \kappa + (\nu + 1 - d)/2 & \text{if } t = 1, r \geq 1, \xi(cq) = 0, \nu \notin 2\mathbf{Z}, 2 \in \mathfrak{p}, \text{ and } \delta = 1, \\ \kappa + [\nu/2] & \text{otherwise.} \end{cases}$$

Thus by (3.11), (3.14), (3.17), and (5.28), we have

(5.59)

$$\varphi[x_1]\mathfrak{g} = \begin{cases} \mathfrak{g} & \text{if } t = 1, r \geq 1, \xi(cq) = 0, \nu \notin 2\mathbf{Z}, 2 \in \mathfrak{p}, \text{ and } \delta = 1, \\ \mathfrak{p}^{\delta} & \text{if } t = 1, r \geq 1, \xi(cq) = -1, \nu \equiv \delta \pmod 2, \text{ and } 2 \in \mathfrak{p}, \\ \mathfrak{p}^{\lambda} & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \text{ and } b\mathfrak{g} = \mathfrak{p}, \\ \mathfrak{p}^{\delta} & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}. \end{cases}$$

Therefore $\mathfrak{r}_E x_1$ is a unique maximal lattice in Ex_1, where $\mathfrak{r}_E$ is the valuation ring of E. Since $N_{E/F}(x_2 x_1^{-1}) = \varphi[x_2]\varphi[x_1]^{-1} \in \mathfrak{g}$, we have $x_2 x_1^{-1} \in \mathfrak{r}_E$. By (5.52) and (5.58), $N_{E/F}(x_2 x_1^{-1} - (x_2 x_1^{-1})^{\rho_E})\mathfrak{g} = D_{E/F}$, where $1 \neq \rho_E \in Gal(E/F)$. Thus [AQC, Lemma 5.6(ii)] implies $\mathfrak{r}_E = \mathfrak{g}[x_2 x_1^{-1}]$, and hence $\mathfrak{g}x_1 + \mathfrak{g}x_2$ is a maximal lattice in Ex_1 in this case.

Next suppose that $t = 1$, $r \geq 1$, $\xi(cq) = 0$, $\nu \in 2\mathbf{Z}$, $2 \in \mathfrak{p}$, and $\delta = 0$. Then $d \in 2\mathbf{Z}$ by Lemma 5.1(3). From this and (5.23), $\tau = \kappa + 2^{-1}(\nu - d)$. Thus $\varphi[x_1]\mathfrak{g} = \mathfrak{p}$ from (3.11) and (5.28). Put $\eta = \pi^{2^{-1}d-\kappa}(1 + \pi^{\tau}\varphi[z]^{-1}wx_1) \in E$, then η is a root of an Eisenstein equation $\mathbf{x}^2 - 2\pi^{2^{-1}d-\kappa}\mathbf{x} - \pi^{d-2\kappa}\varphi[z]^{-1}(q - \varphi[z]) = 0$. Here $\mathbf{x}$ is an indeterminate. Therefore η is a prime element of E and $(\eta - \eta^{\rho_E})\mathfrak{r}_E = (2\eta - 2\pi^{2^{-1}d-\kappa})\mathfrak{r}_E = \mathfrak{d}_{E/F}$. Here $\mathfrak{r}_E$ and ρ_E are the same symbols as above. Thus $\mathfrak{r}_E = \mathfrak{g}[\eta]$ by [AQC, Lemma 5.6(ii)]. From $\varphi[x_1]\mathfrak{g} = \mathfrak{p}$, we have $\Lambda = \mathfrak{r}_E \eta^{-1} x_1 = \mathfrak{g}x_1 + \mathfrak{g}\eta^{-1}x_1$ with Λ of (5.50). Since $\eta^{-1} = -\pi^{\kappa - 2^{-1}d}\varphi[z](q - \varphi[z])^{-1}(1 - \pi^{\tau}\varphi[z]^{-1}wx_1)$, we obtain $\Lambda = \mathfrak{g}x_1 + \mathfrak{g}x_2$. This proves (5.56).

Now, we obtain (5.55) when $t = 1$, $r \geq 1$, $\nu \equiv \delta \pmod 2$, $\xi(cq) \neq 1$, and $2 \in \mathfrak{p}$ by (5.56). When $t > 1$, we have

(5.60)

$$[(\mathfrak{g}x_1 + \mathfrak{g}x_2)\tilde{} : \mathfrak{g}x_1 + \mathfrak{g}x_2] = \begin{cases} [\mathfrak{g} : \mathfrak{p}^{2\lambda}] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \text{ and } b\mathfrak{g} = \mathfrak{p}, \\ [\mathfrak{g} : \mathfrak{p}^{2\delta}] & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}. \end{cases}$$

by (5.56), (5.57), (5.58), (5.59), and [AQC, Lemma 8.4(iv)]. Put

$$\Lambda_Y = \begin{cases} \mathfrak{g}y & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \text{ and } b\mathfrak{g} = \mathfrak{p}, \\ \mathfrak{r}_Y y_2 & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}. \end{cases}$$

Then Λ_Y is maximal in Y. Indeed, if $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b\mathfrak{g} = \mathfrak{p}$, then $\dim_F(Fy) = 1$. We have $\varphi[y]\mathfrak{g} = \mathfrak{p}^{1-\lambda}$ from (5.31) and

(5.34), and hence $\mathfrak{g}y$ is maximal in Y by [AQC, Lemma 6.4]. If $t = 3$, $r \geq 1$, $\xi(-cq) = 1$, and $2 \in \mathfrak{p}$, then K_Y in (5.43) is unramified over F and $Y = K_Y y_2$. Also we have $\varphi[ky_2] = \varphi[y_2]N_{K_Y/F}(k)$ for $k \in K_Y$. Thus $\mathfrak{r}_Y y_2$ is maximal in Y by (5.45) and [AQC, Lemma 6.4]. Since Λ_Y is maximal in Y, [AQC, Lemma 8.4(iv)] and Lemma 5.2 imply

$$[\widetilde{\Lambda_Y} : \Lambda_Y] = \begin{cases} [\mathfrak{g} : 2\mathfrak{p}^{1-\lambda}] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \text{ and } b\mathfrak{g} = \mathfrak{p}, \\ [\mathfrak{g} : \mathfrak{p}^{2(1-\delta)}] & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}. \end{cases}$$

Combining this with (5.60), we obtain

$$\begin{aligned} [(\mathfrak{g}x_1 + \mathfrak{g}x_2 + \Lambda_Y)\widetilde{} : \mathfrak{g}x_1 + \mathfrak{g}x_2 + \Lambda_Y] &= [(\mathfrak{g}x_1 + \mathfrak{g}x_2)\widetilde{} : \mathfrak{g}x_1 + \mathfrak{g}x_2] \cdot [\widetilde{\Lambda_Y} : \Lambda_Y] \\ &= \begin{cases} [\mathfrak{g} : 2\mathfrak{p}^{1+\lambda}] & \text{if } t = 2, r \geq 1, c^{-1}q \notin N_{K/F}(\mathfrak{r}), d > 1, \\ & \qquad \text{and } b\mathfrak{g} = \mathfrak{p}, \\ [\mathfrak{g} : \mathfrak{p}^2] & \text{if } t = 3, r \geq 1, \xi(-cq) = 1, \text{ and } 2 \in \mathfrak{p}. \end{cases} \end{aligned}$$

Therefore $\mathfrak{g}x_1 + \mathfrak{g}x_2 + \Lambda_Y$ is maximal in X by [AQC, Lemma 8.4(iv)] and Lemma 5.2. Note that $\varphi[x_1]\varphi[w]\varphi[y]\mathfrak{g} = \mathfrak{p}^{\nu-2\kappa+1}$ by (5.34), (5.53), and (5.59), when $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b\mathfrak{g} = \mathfrak{p}$. Therefore we obtain (5.55).

5.14. Finally, we suppose that $t = 2$, $r \geq 1$, $c^{-1}q \notin N_{K/F}(\mathfrak{r})$, $d > 1$, and $b \in \mathfrak{g}^\times$. We have already obtained

$$H = \mathfrak{g}\pi^{\tau-i}x_1 + \mathfrak{g}x_3 + \mathfrak{g}y \tag{5.61}$$

by (5.48), with x_1 of (5.27), y satisfying (5.34), and x_3 of (5.49). Our aim is to show that H coincides with the unique maximal lattice Λ in X if and only if $i = \tau$, with Λ of (5.50). For the purpose, we shall find a $\mathfrak{g}$-basis of Λ in a similar way as §2.3(III) (cf. (2.19)).

We consider the Clifford algebra $A(X)$ of the restriction of φ to X. Put

$$x_0 = \pi^{\lambda-1}x_1 \text{ and } w_0 = \pi^{-(\nu-d+\lambda)/2}w$$

with λ of (5.35) and w of (5.51). Then $\{x_0, w_0, y\}$ is an F-basis of X satisfying $\varphi(x_0, w_0) = \varphi(w_0, y) = \varphi(y, x_0) = 0$ by (5.54) and $Y = Fy$ with Y in (5.31). Thus we obtain

$$X = T_X\zeta_X \text{ and } \varphi[x\zeta_X] = c_X N_{B/F}(x) \text{ for } x \in T_X.$$

Here

$$T_X = Fx_0w_0 + Fx_0y + Fw_0y, B = F + T_X, c_X = \varphi[x_0]\varphi[w_0]\varphi[y], \zeta_X = x_0w_0y.$$

Note that B is a division quaternion algebra over F. Moreover we have $c_X\mathfrak{g} = \mathfrak{p}^\lambda$ by (5.28), (5.34), and (5.53). Therefore

$$\Lambda = (T_X \cap \mathfrak{P}^{-\lambda})\zeta_X, \tag{5.62}$$

where $\mathfrak{P} = \{x \in B \mid N_{B/F}(x) \in \mathfrak{p}\}$. Put

$$\omega_X = -x_1\zeta_X^{-1}, u_X = x_3\zeta_X^{-1}\omega_X^{-1}, \text{ and } v_X = u_X - u_X^\iota \tag{5.63}$$

in B, where ι is the main involution of B. Then we assert that

$$\Lambda = [\mathfrak{g}v_X + (\mathfrak{g} + \mathfrak{g}u_X)\omega_X]\zeta_X = \mathfrak{g}x_1 + \mathfrak{g}x_3 + \mathfrak{g}v_X\zeta_X. \tag{5.64}$$

Indeed, we have $\omega_X^2\mathfrak{g} = \mathfrak{p}^{1-2\lambda}$ by (5.34) and (5.53). Thus we obtain

$$\begin{aligned} N_{B/F}(u_X) &= c_X^{-1}N_{B/F}(\omega_X)^{-1}\pi^{d-2\kappa-2\lambda}\varphi[y](-\pi^{2\kappa+1-d}\beta) \in \mathfrak{g}^\times, \\ N_{B/F}(v_X) &= N_{B/F}(u_X - u_X^\iota) \\ &= 4\pi^{-2\lambda+d-2\kappa}\varphi[x_1]^{-1}\varphi[y](s + \pi^{2\kappa+1-d}\beta)(s-1)^{-1} \in \mathfrak{g}^\times \end{aligned}$$

by (5.28), (5.34), (5.38), (5.49), and (5.53). Note that $2\kappa+1 > d$ by $d > 1$ and Lemma 4.2. Thus [AQC, Lemma 5.6(ii)] implies that $F + Fu_X$ is an unramified quadratic extension of F and $\mathfrak{g} + \mathfrak{g}u_X$ is the valuation ring of $F + Fu_X$. Also we have $v_X \in \mathfrak{g}[u_X]^\times$. We see that $B = (F + Fu_X) + (F + Fu_X)\omega_X$ and $v_X\omega_X = -\omega_Xv_X$ by a straightforward caluculation. Combining these with (5.62), we obtain the first equality of (5.64) in the same way as §2.3(III). The second equality of (5.64) is trivial from (5.63). This proves (5.64).

Now, we consider the $\mathfrak{g}$-base of both H and Λ, that is, $\{\pi^{\tau-i}x_1, x_3, y\}$ and $\{x_1, x_3, v_X\zeta_X\}$; see (5.61) and (5.64) above. We see that

$$\begin{aligned} v_X\zeta_X &= 2\pi^{d-\kappa-1-(\nu+\lambda)/2}\varphi[y][w + (-1)^{\nu+1}\pi^{-(\nu+\lambda)/2}\alpha\varphi[w]y] \\ &= A(\pi^{\tau-i}x_1) + Bx_3 + Cy \end{aligned}$$

with

$$\begin{aligned} A &= -2\varphi[y]\varphi[z](q - \varphi[z])^{-1}\pi^{i+d-\kappa-1-(\nu+\lambda)/2} \in \mathfrak{p}^{i-\tau}, \\ B &= (-1)^\nu 2\alpha^{-1}\pi^{\lambda-1+2^{-1}d} \in \mathfrak{g}, \\ C &= (-1)^{\nu+1}2\pi^{d-\kappa-1}(\alpha^{-1} + \alpha\varphi[y]\varphi[w]\pi^{-\nu-\lambda}) \in \mathfrak{g}^\times \end{aligned}$$

by (5.23), (5.34), (5.38), (5.53), and $d > 1$. Thus

$$(\pi^{\tau-i}x_1, x_3, y) = (x_1, x_3, v_X\zeta_X)\gamma, \quad \gamma = \begin{bmatrix} \pi^{\tau-i} & 0 & -\pi^{\tau-i}AC^{-1} \\ 0 & 1 & -BC^{-1} \\ 0 & 0 & C^{-1} \end{bmatrix}.$$

Since $\gamma \in \mathfrak{g}_3^3$ and $\det(\gamma)\mathfrak{g} = \mathfrak{p}^{\tau-i}$, we obtain $H = \Lambda$ if and only if $i = \tau$, also in this case. This completes the proof.

6 GLOBAL RESULTS

In this section we assume that F is a global field and L is a maximal lattice in V with respect to φ. We state two global results which are derived from the local cases.

6.1. Let $\mathbf{h}$ be the set of nonarchmedean primes of F and fix $v \in \mathbf{h}$. We let F_v denote the completion of F at v. Then F_v is a local field. Let $\mathfrak{g}_v$ be the valuation ring of F_v and $\mathfrak{p}_v$ the maximal ideal of $\mathfrak{g}_v$. We also write $\mathfrak{p}_v$ for the prime ideal of $\mathfrak{g}$ corresponding to v. Put $X_v = X \otimes_F F_v$ for a subspace X of V and $\Lambda_v = \Lambda \otimes_{\mathfrak{g}} \mathfrak{g}_v$ for a $\mathfrak{g}$-lattice Λ in V. Let φ_v be the F_v-bilinear extension of φ to $V_v \times V_v$. We consider (V_v, φ_v). By [AQC, Lemma 9.4(iii)], L_v is a maximal lattice in V_v. For $q \in \mathfrak{g} \cap F^\times$ such that $L_v[q] \neq \emptyset$, put

$$\tau_v(q) = \max(\{i \in \mathbf{Z} \mid L_v[q] \supset L_v[q, 2^{-1}\mathfrak{p}_v^i] \neq \emptyset\}). \tag{6.1}$$

This is given by (3.9), (3.12), (3.15), (3.18), and (3.20) for every $v \in \mathbf{h}$.

6.2 Proposition. *Let the notation be as above. Let L be a maximal lattice in V and $q \in \mathfrak{g} \cap F^\times$. Let t_v be the core dimension of (V_v, φ_v) for $v \in \mathbf{h}$. Put $n = \dim_F(V)$. Then for a $\mathfrak{g}$-ideal $\mathfrak{a} = \prod_{v \in \mathbf{h}} \mathfrak{p}_v^{i_v}$ such that $\mathfrak{a} \subset \mathfrak{g}$, we have*

$$L[q, 2^{-1}\mathfrak{a}] \neq \emptyset \Longrightarrow \begin{cases} i_v = \tau_v(q) & \text{if } n = t_v, \\ i_v \leq \tau_v(q) & \text{otherwise} \end{cases}$$

for all $v \in \mathbf{h}$.

Proof. Assume $L[q, 2^{-1}\mathfrak{a}] \neq \emptyset$. For every $v \in \mathbf{h}$, we have $L[q, 2^{-1}\mathfrak{a}] \subset L_v[q, 2^{-1}\mathfrak{p}_v^{i_v}]$ since $\varphi(x, L)_v = \varphi_v(x, L_v)$ for any $x \in V$. Thus we obtain $\emptyset \neq L_v[q, 2^{-1}\mathfrak{p}_v^{i_v}] \subset L_v[q]$ by Lemma 3.6, and hence Corollary 3.7 implies the assertion. □

6.3 Theorem. *Let the notation be the same as in Proposition 6.2. Let L be a maximal lattice in V. Assume $n \geq 2$. Then for $h \in L$ such that $\varphi[h] \neq 0$, we have*

$$L \cap (Fh)^\perp \text{ is maximal in } (Fh)^\perp \Longleftrightarrow h \in L\big[\varphi[h], 2^{-1} \prod_{v \in \mathbf{h}} \mathfrak{p}_v^{\tau_v(\varphi[h])}\big].$$

Here $(Fh)^\perp = \{x \in V \mid \varphi(x, h) = 0\}$.

Proof. Put $W = (Fh)^\perp$. Then we see that $W_v = (F_v h)^\perp$ in V_v for all $v \in \mathbf{h}$. By [AQC, Lemma 9.4(iii)], $L \cap W$ is maximal in W if and only if $L_v \cap W_v = (L \cap W)_v$ is maximal in W_v for every $v \in \mathbf{h}$; Moreover Theorem 5.3 shows that this is the case if and only if $h \in L_v\big[\varphi[h], 2^{-1}\mathfrak{p}_v^{\tau_v(\varphi[h])}\big]$ for all $v \in \mathbf{h}$. Since $\varphi(h, L)_v = \varphi_v(h, L_v)$, the assertion holds. □

This theorem answers the question raised in [AQC, (11.6a)].

7 Sums of squares

7.1. Put $V = \mathbf{Q}_n^1$ and $\varphi(x, y) = x \cdot {}^t y$ for $x, y \in V$. Let L be a maximal lattice in V and $\{e_i\}_{i=1}^n$ the standard $\mathbf{Q}$-basis of V in this section. Then $\varphi[x] = \sum_{i=1}^n x_i^2$

for $x = \sum_{i=1}^{n} x_i e_i \in V$. Hereafter we assume that q is a squarefree positive integer. By [AQC, (12.17)],

$$L[q] = L[q, 2^{-1}\mathbf{Z}] \sqcup L[q, \mathbf{Z}].$$

Here we apply our results on $L[q]$ in this case and investigate the sets $L[q, 2^{-1}\mathbf{Z}]$ and $L[q, \mathbf{Z}]$ when $4 \le n \le 10$ and $n \in 2\mathbf{Z}$. As for the case $n \notin 2\mathbf{Z}$, we can refer to [AQC, Section 12].

7.2 LEMMA. *Assume $n \ge 4$. Let L be a maximal lattice in V and q a squarefree positive integer. Then*

$$L[q, \mathbf{Z}] = \emptyset \textit{ if } \begin{cases} n \equiv 0 \pmod 8; \textit{ or} \\ n \equiv \pm 1 \pmod 8 \textit{ and } (-1)^{(n-1)/2} q \not\equiv 1 \pmod 4; \textit{ or} \\ n \equiv \pm 2 \pmod 8 \textit{ and } (-1)^{(n-2)/4} q \equiv 3 \pmod 4; \textit{ or} \\ n \equiv 4 \pmod 8 \textit{ and } q \equiv 1 \pmod 2 \end{cases}$$

and $L[q, 2^{-1}\mathbf{Z}] = \emptyset$ *if* $n = 4$ *and* $q \equiv 0 \pmod 2$.

Proof. Let p be a rational prime number. The core dimension t_p of (V_p, φ_p) is given by [AQC, (7.12a) and (7.12b)]. Let c_p be as in §2.3 when $1 \le t_p \le 3$. By a Witt decomposition of V_p as in (2.4), we have $(-1)^{(n-t_p)/2} c_p \mathbf{Q}_p^{\times 2} = \delta(V_p, \varphi_p) = \mathbf{Q}_p^{\times 2}$ for $t_p = 1, 3$. From this and [AQC, §7.15], we can take c_p so that $c_p \in \mathbf{Z}_p^{\times}$ when $p \ne 2$ and

$$c_2 = \begin{cases} (-1)^{(n-t_2)/2} & \text{if } t_2 = 1, 3, \\ (-1)^{(n-2)/4} & \text{if } t_2 = 2 \end{cases}$$

when $p = 2$. Let $\tau_p(q)$ be as in (6.1). Then we see that

$$\tau_p(q) = \begin{cases} 1 & \text{if } n \equiv \pm 1 \pmod 8, p = 2, \text{ and } (-1)^{(n-1)/2} q \equiv 1 \pmod 4; \\ & \text{or } n \equiv \pm 2 \pmod 8, p = 2, \text{ and } (-1)^{(n-2)/4} q \not\equiv 3 \pmod 4; \\ & \text{or } n \equiv \pm 3 \pmod 8 \text{ and } p = 2; \\ & \text{or } n \equiv 4 \pmod 8, p = 2, \text{ and } q \equiv 0 \pmod 2), \\ 0 & \text{otherwise} \end{cases} \tag{7.1}$$

by Theorem 3.5 and Lemma 4.2(1). Note that $N_{\mathbf{Q}(\sqrt{-1})_2/\mathbf{Q}_2}(\mathbf{Z}[\sqrt{-1}]_2^{\times}) = (1 + 4\mathbf{Z}_2)\mathbf{Z}_2^{\times 2}$. Combining (7.1) with Proposition 6.2, the assertion holds. □

If $n \equiv \pm 1 \pmod 8$, then this lemma is a restatement of [AQC, Lemma 12.13(ii)].

7.3. Put

$$L_n = \mathbf{Z}e_1 + \mathbf{Z}e_2 + \sum_{i=2}^{n/2} (\mathbf{Z}e_{2i-1} + \mathbf{Z}g_{2i}) \tag{7.2}$$

for $4 \leq n \equiv 2, 4, 6 \pmod 8$, where $g_{2i} = 2^{-1}(e_{2i-3} + e_{2i-2} + e_{2i-1} + e_{2i})$. Then L_n is maximal in V by [CGQ, Lemma 3.1]. When $n = 10$, we put

$$\Lambda = H + M \tag{7.3}$$

with a maximal lattice H (resp. M) in $\sum_{i=1}^{8} \mathbf{Q}e_i$ (resp. $\mathbf{Q}e_9 + \mathbf{Q}e_{10}$). Then Λ is a maximal lattice in V by [NRQ, §6.8]. Hereafter we suppose $4 \leq n \leq 10$ and $n \in 2\mathbf{Z}$. By [AQC, §12.12], if $n < 10$, then the genus $LSO^{\varphi}_{\mathbf{A}}$ of L (cf. [AQC, §§9.3 and 9.7]) equals to the SO^{φ}-class LSO^{φ}. Here $SO^{\varphi}_{\mathbf{A}}$ is the adelization of SO^{φ}. If $n = 10$, then [CGQ, §3.2] and [AQC, Lemma 9.23(i)] imply $LSO^{\varphi}_{\mathbf{A}} = L_{10}SO^{\varphi} \sqcup \Lambda SO^{\varphi}$.

7.4 Lemma. *Let L_n be as in (7.2) and q a squarefree positive integer. Assume $n = 4, 6$, or 10. Then we obtain the following assertions:*

(1)*Assume $n = 4$. Then we have $L_4[q, 2^{-1}\mathbf{Z}] = \emptyset$ if and only if $q \equiv 0 \pmod 2$ and $L_4[q, \mathbf{Z}] = \emptyset$ if and only if $q \equiv 1 \pmod 2$.*
(2) *If $n > 4$, then $L_n[q, 2^{-1}\mathbf{Z}] \neq \emptyset$.*
(3) *If $n > 4$ and $q \equiv 0 \pmod 2$, then $L_n[q, \mathbf{Z}] \neq \emptyset$.*
(4) *If $n = 6$ and $q \equiv 3 \pmod 4$, then $L_6[q, \mathbf{Z}] \neq \emptyset$.*
(5) *Assume $n = 10$ and $q \equiv 1 \pmod 4$. Then we have $L_{10}[q, \mathbf{Z}] = \emptyset$ if and only if $q = 1$.*

Proof. (1): Assume $n = 4$. Since L_4 is maximal in V,

$$L_4[q] = \begin{cases} L_4[q, 2^{-1}\mathbf{Z}] & \text{if } q \equiv 1 \pmod 2, \\ L_4[q, \mathbf{Z}] & \text{if } q \equiv 0 \pmod 2 \end{cases}$$

by Lemma 7.2. We have $\sum_{i=1}^{4} \mathbf{Z}e_i \subset L_4$, and hence

$$L_4[q] \neq \emptyset \text{ for any squarefree positive integer } q. \tag{7.4}$$

This proves (1). (2): Assume $n > 4$. We can take $x \in L_4$ so that $\varphi[x] = q$ or $q - 1$ according as $q \equiv 1 \pmod 2$ or $q \equiv 0 \pmod 2$ by (7.4). If $q \equiv 1 \pmod 2$, then put $h = x$; if $q \equiv 0 \pmod 2$, then put $h = x + e_5$. By (1) settled above, $h \in L_n[q, 2^{-1}\mathbf{Z}]$ in both cases. This proves (2). In the proof of (3) and (4) we take

$$y = \sum_{i=1}^{4} y_i e_i \in \sum_{i=1}^{4} \mathbf{Z}e_i \text{ such that } \varphi[y] = q \tag{7.5}$$

for a given q. (3): Suppose $n > 4$ and $q \equiv 0 \pmod 2$. Since q is even and squarefree, at least two of y_1, y_2, y_3, and y_4 are even. We may assume $y_3, y_4 \in 2\mathbf{Z}$. Then $y \in L_n[q, \mathbf{Z}]$ from (1). This proves (3). Now, for $h = \sum_{i=1}^{n} h_i e_i \in V$ such that $\varphi[h] = q$, we have

$$h \in L_n[q, \mathbf{Z}] \Longleftrightarrow h \in \sum_{i=1}^{n} \mathbf{Z}e_i \text{ and } \sum_{k=0}^{3} h_{2j-k} \in 2\mathbf{Z} \text{ for } 2 \leq j \leq n/2. \tag{7.6}$$

(4): Suppose $n = 6$ and $q \equiv 3 \pmod 4$. Then one and only one of y_1, y_2, y_3, and y_4 in (7.5) is even. We may assume $y_1 \in 2\mathbf{Z}$. Put $h = \sum_{i=1}^{3} y_i e_i + y_4 e_5$, then $h \in L_6[q, \mathbf{Z}]$ by (7.6). This proves (4). (5): Assume $n = 10$ and $q \equiv 1 \pmod 4$. Then $L_{10}[1, \mathbf{Z}] = \emptyset$ by (7.6). If $q > 1$, then there exists $z = \sum_{i=1}^{4} z_i e_i \in \sum_{i=1}^{4} \mathbf{Z} e_i$ such that $\sum_{i=1}^{4} z_i^2 = 4^{-1}(q-5)$. Put $h = \sum_{i=1}^{4} 2z_i e_{2i} + \sum_{j=1}^{5} e_{2j-1}$. Then $h \in L_{10}[q, \mathbf{Z}]$ by (7.6). This completes the proof. $\square$

7.5 THEOREM. *Let L be a maximal lattice in V and q a squarefree positive integer. We assume $4 \le n \le 10$ and $n \in 2\mathbf{Z}$. Then*

$$L[q, \mathbf{Z}] = \emptyset \text{ if and only if } \begin{cases} n = 4 \text{ and } q \equiv 1 \pmod 2; \text{ or} \\ n = 6 \text{ and } q \equiv 1 \pmod 4; \text{ or} \\ n = 8; \text{ or} \\ n = 10, L \in L_{10} SO^{\varphi}, q = 1 \text{ or } q \equiv 3 \pmod 4; \text{ or} \\ n = 10, L \in \Lambda SO^{\varphi}, q \equiv 3 \pmod 4 \end{cases}$$

and $L[q, 2^{-1}\mathbf{Z}] = \emptyset$ if and only if $n = 4$ and $q \equiv 0 \pmod 2$. Here L_{10} (resp. Λ) is of (7.2) (resp. (7.3)).

Proof. If $n = 4, 6$, or, $n = 10$ and $LSO^{\varphi} = L_{10} SO^{\varphi}$, then we have $LSO^{\varphi} = L_n SO^{\varphi}$. Therefore we obtain the assertion by Lemma 7.2 and Lemma 7.4. Assume $n = 8$. Then Lemma 7.2 implies $L[q] = L[q, 2^{-1}\mathbf{Z}]$. By [AQC, Lemma 6.2(1)], we may assume $\sum_{i=1}^{4} \mathbf{Z} e_i \subset L$, and hence $L[q] \neq \emptyset$. This proves our theorem in the case $n = 8$. Next assume $n = 10$ and $LSO^{\varphi} = \Lambda SO^{\varphi}$. Then we may put $L = \Lambda$. For $x = h + m \in H + M = \Lambda$, we have $\varphi[x] = \varphi[h] + \varphi[m]$ and $\varphi(x, \Lambda) = \varphi(h, H) + \varphi(m, M)$. Thus we obtain $H[q, 2^{-1}\mathbf{Z}] \subset \Lambda[q, 2^{-1}\mathbf{Z}]$. From this and the result of the case $n = 8$, we have $\Lambda[q, 2^{-1}\mathbf{Z}] \neq \emptyset$. Next we consider $\Lambda[q, \mathbf{Z}]$. We see that $L_6 + \mathbf{Z} f_7 + \mathbf{Z} g_8$ (resp. $\mathbf{Z} e_9 + \mathbf{Z} e_{10}$) is maximal in $\sum_{i=1}^{8} \mathbf{Q} e_i$ (resp. $\mathbf{Q} e_9 + \mathbf{Q} e_{10}$) by [CGQ, Lemma 3.1]. Here L_6 and g_8 are given in (7.2) and $f_7 = 2^{-1}(e_1 + e_3 + e_5 + e_7)$. Thus we can put

$$\Lambda = H + M = L_6 + \mathbf{Z} f_7 + \mathbf{Z} g_8 + \mathbf{Z} e_9 + \mathbf{Z} e_{10}.$$

Then, for $x = \sum_{i=1}^{10} x_i e_i \in V$ such that $\varphi[h] = q$, we have

(7.7)

$$x \in \Lambda[q, \mathbf{Z}] \Longleftrightarrow x \in \sum_{i=1}^{10} \mathbf{Z} e_i, \ \sum_{k=0}^{3} x_{2k+1} \in 2\mathbf{Z}, \ \sum_{k=0}^{3} x_{2j-k} \in 2\mathbf{Z} \text{ for } 2 \le j \le 4.$$

Assuming $q \not\equiv 3 \pmod 4$, we take y so that (7.5). Then at least two of y_1, y_2, y_3, and y_4 are even. We may assume $y_1, y_2 \in 2\mathbf{Z}$. Put $h = y_1 e_1 + y_2 e_2 + y_3 e_9 + y_4 e_{10}$, then $h \in \Lambda[q, \mathbf{Z}]$ by (7.7). Therefore if $\Lambda[q, \mathbf{Z}] = \emptyset$, then $q \equiv 3 \pmod 4$. Combining this with Lemma 7.2, we obtain our theorem. $\square$

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The Index of Centralizers of Elements of Reductive Lie Algebras

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Abstract. For a finite dimensional complex Lie algebra, its index is the minimal dimension of stabilizers for the coadjoint action. A famous conjecture due to A.G. Elashvili says that the index of the centralizer of an element of a reductive Lie algebra is equal to the rank. That conjecture caught attention of several Lie theorists for years. It reduces to the case of nilpotent elements. In [Pa03a] and [Pa03b], D.I. Panyushev proved the conjecture for some classes of nilpotent elements (e.g. regular, subregular and spherical nilpotent elements). Then the conjecture has been proven for the classical Lie algebras in [Y06a] and checked with a computer programme for the exceptional ones [deG08]. In this paper we give an almost general proof of that conjecture.

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1. Introduction

In this note $\Bbbk$ is an algebraically closed field of characteristic 0.

1.1. Let $\mathfrak{g}$ be a finite dimensional Lie algebra over $\Bbbk$ and consider the coadjoint representation of $\mathfrak{g}$. By definition, the *index* of $\mathfrak{g}$ is the minimal dimension of stabilizers $\mathfrak{g}^x$, $x \in \mathfrak{g}^*$, for the coadjoint representation:

$$\operatorname{ind}\mathfrak{g} := \min\{\dim \mathfrak{g}^x;\ x \in \mathfrak{g}^*\}.$$

The definition of the index goes back to Dixmier [Di74]. It is a very important notion in representation theory and in invariant theory. By Rosenlicht's theorem [Ro63], generic orbits of an arbitrary algebraic action of a linear algebraic group on an irreducible algebraic variety are separated by rational invariants; in particular, if $\mathfrak{g}$ is an algebraic Lie algebra,

$$\operatorname{ind}\mathfrak{g} = \deg\operatorname{tr}\Bbbk(\mathfrak{g}^*)^{\mathfrak{g}},$$

where $\Bbbk(\mathfrak{g}^*)^{\mathfrak{g}}$ is the field of $\mathfrak{g}$-invariant rational functions on $\mathfrak{g}^*$. The index of a reductive algebra equals its rank. For an arbitrary Lie algebra, computing its index seems to be a wild problem. However, there is a large number of interesting results for several classes of nonreductive subalgebras of reductive Lie algebras. For instance, parabolic subalgebras and their relatives as nilpotent radicals, seaweeds, are considered in [Pa03a], [TY04], [J07]. The centralizers, or normalizers of centralizers, of elements form another interesting class of such subalgebras, [E85a], [Pa03a], [Mo06b]. The last topic is closely related to the theory of integrable Hamiltonian systems [Bol91]. Let us precise this link.

From now on, $\mathfrak{g}$ is supposed to be reductive. Denote by G the adjoint group of $\mathfrak{g}$. The symmetric algebra $\mathrm{S}(\mathfrak{g})$ carries a natural Poisson structure. By the so-called *argument shift method*, for x in $\mathfrak{g}^*$, we can construct a Poisson-commutative family $\mathcal{F}_x$ in $\mathrm{S}(\mathfrak{g}) = \Bbbk[\mathfrak{g}^*]$; see [MF78] or Remark 1.4. It is generated by the derivatives of all orders in the direction $x \in \mathfrak{g}^*$ of all elements of the algebra $\mathrm{S}(\mathfrak{g})^{\mathfrak{g}}$ of $\mathfrak{g}$-invariants of $\mathrm{S}(\mathfrak{g})$. Moreover, if $G.x$ denotes the coadjoint orbit of $x \in \mathfrak{g}^*$:

Theorem 1.1 ([Bol91], Theorems 2.1 and 3.2). *There is a Poisson-commutative family of polynomial functions on $\mathfrak{g}^*$, constructed by the argument shift method, such that its restriction to $G.x$ contains $\frac{1}{2}\dim(G.x)$ algebraically independent functions if and only if* $\operatorname{ind}\mathfrak{g}^x = \operatorname{ind}\mathfrak{g}$.

Denote by $\operatorname{rk}\mathfrak{g}$ the rank of $\mathfrak{g}$. Motivated by the preceding result of Bolsinov, A.G. Elashvili formulated a conjecture:

Conjecture 1.2 (Elashvili). *Let $\mathfrak{g}$ be a reductive Lie algebra. Then* $\operatorname{ind}\mathfrak{g}^x = \operatorname{rk}\mathfrak{g}$ *for all $x \in \mathfrak{g}^*$.*

Elashvili's conjecture also appears in the following problem: Is the algebra $\mathrm{S}(\mathfrak{g}^x)^{\mathfrak{g}^x}$ of invariants in $\mathrm{S}(\mathfrak{g}^x)$ under the adjoint action a polynomial algebra? This question was formulated by A. Premet in [PPY07, Conjecture 0.1]. After that, O. Yakimova discovered a counterexample [Y07], but the question remains very interesting. As an example, under certain hypothesis and under the condition that Elashvili's conjecture holds, the algebra of invariants $\mathrm{S}(\mathfrak{g}^x)^{\mathfrak{g}^x}$ is polynomial in $\operatorname{rk}\mathfrak{g}$ variables, [PPY07, Theorem 0.3].

During the last decade, Elashvili's conjecture caught attention of many invariant theorists [Pa03a], [Ch04], [Y06a], [deG08]. To begin with, describe some easy but useful reductions. Since the $\mathfrak{g}$-modules $\mathfrak{g}$ and $\mathfrak{g}^*$ are

isomorphic, it is equivalent to prove Conjecture 1.2 for centralizers of elements of $\mathfrak{g}$. On the other hand, by a result due to E.B. Vinberg [Pa03a], the inequality $\mathrm{ind}\,\mathfrak{g}^x \geq \mathrm{rk}\,\mathfrak{g}$ holds for all $x \in \mathfrak{g}$. So it only remains to prove the opposite one. Given $x \in \mathfrak{g}$, let $x = x_{\mathrm{s}} + x_{\mathrm{n}}$ be its Jordan decomposition. Then $\mathfrak{g}^x = (\mathfrak{g}^{x_{\mathrm{s}}})^{x_{\mathrm{n}}}$. The subalgebra $\mathfrak{g}^{x_{\mathrm{s}}}$ is reductive of rank $\mathrm{rk}\,\mathfrak{g}$. Thus, the verification of Conjecture 1.2 reduces to the case of nilpotent elements. At last, one can clearly restrict oneself to the case of simple $\mathfrak{g}$.
Review now the main results obtained so far on Elashvili's conjecture. If x is regular, then $\mathfrak{g}^x$ is a commutative Lie algebra of dimension $\mathrm{rk}\,\mathfrak{g}$. So, Conjecture 1.2 is obviously true in that case. Further, the conjecture is known for subregular nilpotent elements and nilpotent elements of height 2 and 3, [Pa03a], [Pa03b]. Remind that the *height* of a nilpotent element e is the maximal integer m such that $(\mathrm{ad}\, e)^m \neq 0$. More recently, O. Yakimova proved the conjecture in the classical case [Y06a]. To valid the conjecture in the exceptional types, W. de Graaf used the computer programme GAP, see [deG08]. Since there are many nilpotent orbits in the Lie algebras of exceptional type, it is difficult to present the results of such computations in a concise way. In 2004, the first author published a case-free proof of Conjecture 1.2 applicable to all simple Lie algebras; see [Ch04]. Unfortunately, the argument in [Ch04] has a gap in the final part of the proof which was pointed out by L. Rybnikov.
To summarize, so far, there is no conceptual proof of Conjecture 1.2. Nevertheless, according to Yakimova's works and de Graaf's works, we can claim:

Theorem 1.3 ([Y06a], [deG08]). *Let $\mathfrak{g}$ be a reductive Lie algebra. Then* $\mathrm{ind}\,\mathfrak{g}^x = \mathrm{rk}\,\mathfrak{g}$ *for all $x \in \mathfrak{g}^*$.*

Because of the importance of Elashvili's conjecture in invariant theory, it would be very appreciated to find a general proof of Theorem 1.3 applicable to all finite-dimensional simple Lie algebras. The proof we propose in this paper is fresh and almost general. More precisely, it remains 7 isolated cases; one nilpotent orbit in type E_7 and six nilpotent orbits in type E_8 have to be considered separately. For these 7 orbits, the use of GAP is unfortunately necessary. In order to provide a complete proof of Theorem 1.3, we include in this paper the computations using GAP we made to deal with these remaining seven cases.

1.2. Description of the paper. Let us briefly explain our approach. Denote by $\mathcal{N}(\mathfrak{g})$ the nilpotent cone of $\mathfrak{g}$. As noticed previously, it suffices to prove $\mathrm{ind}\,\mathfrak{g}^e = \mathrm{rk}\,\mathfrak{g}$ for all e in $\mathcal{N}(\mathfrak{g})$. If the equality holds for e, it

does for all elements of $G.e$; we shortly say that $G.e$ satisfies Elashvili's conjecture.
From a nilpotent orbit $\mathcal{O}_{\mathfrak{l}}$ of a reductive factor $\mathfrak{l}$ of a parabolic subalgebra of $\mathfrak{g}$, we can construct a nilpotent orbit of $\mathfrak{g}$ having the same codimension in $\mathfrak{g}$ as $\mathcal{O}_{\mathfrak{l}}$ in $\mathfrak{l}$ and having other remarkable properties. The nilpotent orbits obtained in such a way are called *induced*; the other ones are called *rigid*. We refer the reader to Subsection 2.3 for more precisions about this topic. Using Bolsinov's criterion of Theorem 1.1, we first prove Theorem 1.3 for all induced nilpotent orbits and so the conjecture reduces to the case of rigid nilpotent orbits. To deal with rigid nilpotent orbits, we use methods developed in [Ch04] by the first author, and resumed in [Mo06a] by the second author, based on nice properties of Slodowy slices of nilpotent orbits.

In more details, the paper is organized as follows:

We state in Section 2 the necessary preliminary results. In particular, we investigate in Subsection 2.2 extensions of Bolsinov's criterion and we establish an important result (Theorem 2.7) which will be used repeatedly in the sequel. We prove in Section 3 the conjecture for all induced nilpotent orbits (Theorem 3.3) so that Elashvili's conjecture reduces to the case of rigid nilpotent orbits (Theorem 3.3). From Section 4, we handle the rigid nilpotent orbits: we introduce and study in Section 4 a property (P) given by Definition 4.2. Then, in Section 5, we are able to deal with almost all rigid nilpotent orbits. Still in Section 5, the remaining cases are dealt with set-apart by using a different approach.

1.3. Notations. • If E is a subset of a vector space V, we denote by $\mathrm{span}(E)$ the vector subspace of V generated by E. The grassmanian of all d-dimensional subspaces of V is denoted by $\mathrm{Gr}_d(V)$. By a *cone* of V, we mean a subset of V invariant under the natural action of $\Bbbk^* := \Bbbk\setminus\{0\}$ and by a *bicone* of $V \times V$ we mean a subset of $V \times V$ invariant under the natural action of $\Bbbk^* \times \Bbbk^*$ on $V \times V$.
• From now on, we assume that $\mathfrak{g}$ is semisimple of rank ℓ and we denote by $\langle .,. \rangle$ the Killing form of $\mathfrak{g}$. We identify $\mathfrak{g}$ to $\mathfrak{g}^*$ through $\langle .,. \rangle$. Unless otherwise specified, the notion of orthogonality refers to the bilinear form $\langle .,. \rangle$.
• Denote by $\mathrm{S}(\mathfrak{g})^{\mathfrak{g}}$ the algebra of $\mathfrak{g}$-invariant elements of $\mathrm{S}(\mathfrak{g})$. Let $f_1, \ldots, f_\ell$ be homogeneous generators of $\mathrm{S}(\mathfrak{g})^{\mathfrak{g}}$ of degrees $d_1, \ldots, d_\ell$ respectively. We choose the polynomials $f_1, \ldots, f_\ell$ so that $d_1 \leq \cdots \leq d_\ell$. For $i = 1, \ldots, \ell$ and $(x, y) \in \mathfrak{g} \times \mathfrak{g}$, we may consider a shift of f_i in direction y: $f_i(x + ty)$ where $t \in \Bbbk$. Expanding $f_i(x + ty)$ as a polynomial

in t, we obtain

$$(1)\qquad f_i(x+ty) = \sum_{m=0}^{d_i} f_i^{(m)}(x,y)t^m; \qquad \forall (t,x,y) \in \Bbbk \times \mathfrak{g} \times \mathfrak{g}$$

where $y \mapsto (m!)f_i^{(m)}(x,y)$ is the differential at x of f_i of the order m in the direction y. The elements $f_i^{(m)}$ as defined by (1) are invariant elements of $\mathrm{S}(\mathfrak{g}) \otimes_{\Bbbk} \mathrm{S}(\mathfrak{g})$ under the diagonal action of G on $\mathfrak{g} \times \mathfrak{g}$. Note that $f_i^{(0)}(x,y) = f_i(x)$ while $f_i^{(d_i)}(x,y) = f_i(y)$ for all $(x,y) \in \mathfrak{g} \times \mathfrak{g}$.

Remark 1.4. The family $\mathcal{F}_x := \{f_i^{(m)}(x,.);\ 1 \leq i \leq \ell, 1 \leq m \leq d_i\}$ for $x \in \mathfrak{g}$, is a Poisson-commutative family of $\mathrm{S}(\mathfrak{g})$ by Mishchenko-Fomenko [MF78]. One says that the family $\mathcal{F}_x$ is constructed by the *argument shift method.*

• Let $i \in \{1,\dots,\ell\}$. For x in $\mathfrak{g}$, we denote by $\varphi_i(x)$ the element of $\mathfrak{g}$ satisfying $(\mathrm{d}f_i)_x(y) = f_i^{(1)}(x,y) = \langle \varphi_i(x), y\rangle$, for all y in $\mathfrak{g}$. Thereby, φ_i is an invariant element of $\mathrm{S}(\mathfrak{g}) \otimes_{\Bbbk} \mathfrak{g}$ under the canonical action of G. We denote by $\varphi_i^{(m)}$, for $0 \leq m \leq d_i - 1$, the elements of $\mathrm{S}(\mathfrak{g}) \otimes_{\Bbbk} \mathrm{S}(\mathfrak{g}) \otimes_{\Bbbk} \mathfrak{g}$ defined by the equality:

$$(2)\qquad \varphi_i(x+ty) = \sum_{m=0}^{d_i-1} \varphi_i^{(m)}(x,y)t^m, \qquad \forall (t,x,y) \in \Bbbk \times \mathfrak{g} \times \mathfrak{g}.$$

• For $x \in \mathfrak{g}$, we denote by $\mathfrak{g}^x = \{y \in \mathfrak{g} \mid [y,x] = 0\}$ the centralizer of x in $\mathfrak{g}$ and by $\mathfrak{z}(\mathfrak{g}^x)$ the center of $\mathfrak{g}^x$. The set of regular elements of $\mathfrak{g}$ is

$$\mathfrak{g}_{\mathrm{reg}} := \{x \in \mathfrak{g} \mid \dim \mathfrak{g}^x = \ell\}$$

and we denote by $\mathfrak{g}_{\mathrm{reg,ss}}$ the set of regular semisimple elements of $\mathfrak{g}$. Both $\mathfrak{g}_{\mathrm{reg}}$ and $\mathfrak{g}_{\mathrm{reg,ss}}$ are G-invariant dense open subsets of $\mathfrak{g}$.
We denote by $C(x)$ the G-invariant cone generated by x and we denote by x_{s} and x_{n} the semisimple and nilpotent components of x respectively.
• The nilpotent cone of $\mathfrak{g}$ is $\mathcal{N}(\mathfrak{g})$. As a rule, for $e \in \mathcal{N}(\mathfrak{g})$, we choose an $\mathfrak{sl}_2$-triple (e,h,f) in $\mathfrak{g}$ given by the Jacobson-Morozov theorem [CMa93, Theorem 3.3.1]. In particular, it satisfies the equalities:

$$[h,e] = 2e, \qquad [e,f] = h, \qquad [h,f] = -2f$$

The action of $\mathrm{a}dh$ on $\mathfrak{g}$ induces a $\mathbb{Z}$-grading:

$$\mathfrak{g} = \bigoplus_{i \in \mathbb{Z}} \mathfrak{g}(i)\ ,\ \mathfrak{g}(i) = \{x \in \mathfrak{g} \mid [h,x] = ix\}.$$

Recall that e, or $G.e$, is said to be *even* if $\mathfrak{g}(i) = 0$ for odd i. Note that $e \in \mathfrak{g}(2)$, $f \in \mathfrak{g}(-2)$ and that $\mathfrak{g}^e$, $\mathfrak{z}(\mathfrak{g}^e)$ and $\mathfrak{g}^f$ are all $\mathrm{a}dh$-stable.

• All topological terms refer to the Zariski topology. If Y is a subset of a topological space X, we denote by $\overline{Y}$ the closure of Y in X.

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Contents

2. Preliminary results

We start in this section by reviewing some facts about the differentials of generators of $\mathrm{S}(\mathfrak{g})^{\mathfrak{g}}$. Then, the goal of Subsection 2.2 is Theorem 2.7. We collect in Subsection 2.3 basic facts about induced nilpotent orbits.

2.1. Differentials of generators of $\mathrm{S}(\mathfrak{g})^{\mathfrak{g}}$. According to subsection 1.3, the elements $\varphi_1,\ldots,\varphi_\ell$ of $\mathrm{S}(\mathfrak{g}) \otimes_{\Bbbk} \mathfrak{g}$ are the differentials of $f_1,\ldots,f_\ell$ respectively. Since $f_i(g(x)) = f_i(x)$ for all $(x,g) \in \mathfrak{g} \times G$, the element $\varphi_i(x)$ centralizes x for all $x \in \mathfrak{g}$. Moreover:

Lemma 2.1. (i)[Ri87, Lemma 2.1] *The elements $\varphi_1(x),\ldots,\varphi_\ell(x)$ belong to $\mathfrak{z}(\mathfrak{g}^e)$.*
(ii)[Ko63, Theorem 9] *The elements $\varphi_1(x),\ldots,\varphi_\ell(x)$ are linearly independent elements of $\mathfrak{g}$ if and only if x is regular. Moreover, if so, $\varphi_1(x),\ldots,\varphi_\ell(x)$ is a basis of $\mathfrak{g}^x$.*

We turn now to the elements $\varphi_i^{(m)}$, for $i = 1,\ldots,\ell$ and $0 \leq m \leq d_i - 1$, defined in Subsection 1.3 by (2). Recall that d_i is the degree of the homogeneous polynomial f_i, for $i = 1,\ldots,\ell$. The integers $d_1-1,\ldots,d_\ell-1$ are thus the exponents of $\mathfrak{g}$. By a classical result [Bou02, Ch. V, §5, Proposition 3], we have $\sum d_i = \mathrm{b}_{\mathfrak{g}}$ where $\mathrm{b}_{\mathfrak{g}}$ is the dimension of Borel subalgebras of $\mathfrak{g}$. For (x,y) in $\mathfrak{g} \times \mathfrak{g}$, we set:

$$V_{x,y} := \mathrm{span}\{\varphi_i^{(m)}(x,y) \ ; \ \ 1 \leq i \leq \ell, 0 \leq m \leq d_i - 1\}. \tag{3}$$

The subspaces $V_{x,y}$ will play a central role throughout the note.

Remark 2.2. (1) For $(x,y) \in \mathfrak{g} \times \mathfrak{g}$, the dimension of $V_{x,y}$ is at most $\mathrm{b}_{\mathfrak{g}}$ since $\sum d_i = \mathrm{b}_{\mathfrak{g}}$. Moreover, for all (x,y) in a nonempty open subset of $\mathfrak{g} \times \mathfrak{g}$, the equality holds [Bol91]. Actually, in this note, we do not need this observation.
(2) By Lemma 2.1(ii), if x is regular, then $\mathfrak{g}^x$ is contained in $V_{x,y}$ for all $y \in \mathfrak{g}$. In particular, if so, $\dim [x, V_{x,y}] = \dim V_{x,y} - \ell$.

The subspaces $V_{x,y}$ were introduced and studied by Bolsinov in [Bol91], motivated by the maximality of Poisson-commutative families in $\mathrm{S}(\mathfrak{g})$. These subspaces have been recently exploited in [PY08] and [CMo08]. The following results are mostly due to Bosinov, [Bol91]. We refer to [PY08] for a more recent account about this topic. We present them in a slightly different way:

Lemma 2.3. *Let (x,y) be in $\mathfrak{g}_{\rm reg} \times \mathfrak{g}$.*
(i) *The subspace $V_{x,y}$ of $\mathfrak{g}$ is the sum of the subspaces $\mathfrak{g}^{x+ty}$ where t runs through any nonempty open subset of $\Bbbk$ such that $x+ty$ is regular for all t in this subset.*
(ii) *The subspace $\mathfrak{g}^y + V_{x,y}$ is a totally isotropic subspace of $\mathfrak{g}$ with respect to the Kirillov form K_y on $\mathfrak{g} \times \mathfrak{g}$, $(v,w) \mapsto \langle y, [v,w]\rangle$. Furthermore, $\dim (\mathfrak{g}^y + V_{x,y})^{\perp} \geq \frac{1}{2} \dim G.y$.*
(iii) *The subspaces $[x, V_{x,y}]$ and $[y, V_{x,y}]$ are equal.*

Proof. (i) Let O be a nonempty open subset of $\Bbbk$ such that $x+ty$ is regular for all t in O. Such an open subset does exist since x is regular. Denote by V_O the sum of all the subspaces $\mathfrak{g}^{x+ty}$ where t runs through O. For all t in O, $\mathfrak{g}^{x+ty}$ is generated by $\varphi_1(x+ty), \ldots, \varphi_\ell(x+ty)$, cf. Lemma 2.1(ii). As a consequence, V_O is contained in $V_{x,y}$. Conversely, for $i = 1, \ldots, \ell$ and for $t_1, \ldots, t_{d_i}$ pairwise different elements of O, $\varphi_i^{(m)}(x,y)$ is a linear combination of $\varphi_i(x+t_1 y), \ldots, \varphi_i(x+t_{d_i} y)$; hence $\varphi_i^{(m)}(x,y)$ belongs to V_O. Thus $V_{x,y}$ is equal to V_O, whence the assertion.
(ii) results from [PY08, Proposition A4]. Notice that in (ii) the inequality is an easy consequence of the first statement.
At last, [PY08, Lemma A2] gives us (iii). □

Let σ and σ_i, for $i = 1, \ldots, \ell$, be the maps

$$\begin{array}{ccc} \mathfrak{g} \times \mathfrak{g} & \stackrel{\sigma}{\longrightarrow} & \Bbbk^{\mathrm{b}_{\mathfrak{g}}+\ell} \\ (x,y) & \longmapsto & (f_i^{(m)}(x,y))_{\substack{1 \leq i \leq \ell, \\ 0 \leq m \leq d_i}} \end{array}, \qquad \begin{array}{ccc} \mathfrak{g} \times \mathfrak{g} & \stackrel{\sigma_i}{\longrightarrow} & \Bbbk^{d_i+1} \\ (x,y) & \longmapsto & (f_i^{(m)}(x,y))_{0 \leq m \leq d_i} \end{array}$$

respectively, and denote by $\sigma'(x,y)$ and $\sigma'_i(x,y)$ the tangent map at (x,y) of σ and σ_i respectively. Then $\sigma'_i(x,y)$ is given by the differentials of the $f_i^{(m)}$'s at (x,y) and $\sigma'(x,y)$ is given by the elements $\sigma'_i(x,y)$.

Lemma 2.4. *Let (x,y) and (v,w) be in $\mathfrak{g}\times\mathfrak{g}$.*
(i) *For $i=1,\ldots,\ell$, $\sigma'_i(x,y)$ maps (v,w) to*

$$(\langle\varphi_i(x),v\rangle, \langle\varphi_i^{(1)}(x,y),v\rangle+\langle\varphi_i^{(0)}(x,y),w\rangle, \\ \ldots, \langle\varphi_i^{(d_i-1)}(x,y),v\rangle+\langle\varphi_i^{(d_i-2)}(x,y),w\rangle, \langle\varphi_i(y),w\rangle).$$

(ii) *Suppose that $\sigma'(x,y)(v,w)=0$. Then, for w' in $\mathfrak{g}$, $\sigma'(x,y)(v,w')=0$ if and only if $w-w'$ is orthogonal to $V_{x,y}$.*
(iii) *For $x\in\mathfrak{g}_{\rm reg}$, $\sigma'(x,y)(v,w')=0$ for some $w'\in\mathfrak{g}$ if and only if $v\in[x,\mathfrak{g}]$.*

Proof. (i) The verifications are easy and left to the reader.
(ii) Since $\sigma'(x,y)(v,w) = 0$, $\sigma'(x,y)(v,w') = 0$ if and only if $\sigma'(x,y)(v,w-w')=0$ whence the statement by (i).
(iii) Suppose that x is regular and suppose that $\sigma'(x,y)(v,w')=0$ for some $w'\in\mathfrak{g}$. Then by (i), v is orthogonal to the elements $\varphi_1(x),\ldots,\varphi_\ell(x)$. So by Lemma 2.1(ii), v is orthogonal to $\mathfrak{g}^x$. Since $\mathfrak{g}^x$ is the orthogonal complement of $[x,\mathfrak{g}]$ in $\mathfrak{g}$, we deduce that v lies in $[x,\mathfrak{g}]$. Conversely, since $\sigma(x,y)=\sigma(g(x),g(y))$ for all g in G, the element $([u,x],[u,y])$ belongs to the kernel of $\sigma'(x,y)$ for all $u\in\mathfrak{g}$. So, the converse implication follows. □

2.2. On Bolsinov's criterion. Let a be in $\mathfrak{g}$ and denote by π the map

$$\begin{array}{ccc}\mathfrak{g}\times G.a & \stackrel{\pi}{\longrightarrow} & \mathfrak{g}\times\Bbbk^{\mathrm{b}_\mathfrak{g}+\ell} \\ (x,y) & \longmapsto & (x,\sigma(x,y)).\end{array}$$

Remark 2.5. Recall that the family $(\mathcal{F}_x)_{x\in\mathfrak{g}}$ constructed by the argument shift method consists of all elements $f_i^{(m)}(x,.)$ for $i=1,\ldots,\ell$ and $1\le m\le d_i$, see Remark 1.4. By definition of the morphism π, there is a family constructed by the argument shift method whose restriction to $G.a$ contains $\frac{1}{2}\dim G.a$ algebraically independent functions if and only if π has a fiber of dimension $\frac{1}{2}\dim G.a$.

In view of Theorem 1.1 and the above remark, we now concentrate on the fibers of π. For $(x,y)\in\mathfrak{g}\times G.a$, denote by $F_{x,y}$ the fiber of π at $\pi(x,y)$:

$$F_{x,y} \;:=\; \{x\}\times\{y'\in G.a \mid \sigma(x,y')=\sigma(x,y)\}.$$

Lemma 2.6. *Let (x,y) be in $\mathfrak{g}\times G.a$.*
(i) *The irreducible components of $F_{x,y}$ have dimension at least* $\frac{1}{2}\dim G.a$.

(ii) *The fiber* $F_{x,y}$ *has dimension* $\frac{1}{2}\dim G.a$ *if and only if any irreducible component of* $F_{x,y}$ *contains an element* (x,y') *such that* $(\mathfrak{g}^{y'}+V_{x,y'})^{\perp}$ *has dimension* $\frac{1}{2}\dim G.a$.

Proof. We prove (i) and (ii) all together. The tangent space $\mathrm{T}_{x,y'}(F_{x,y})$ of $F_{x,y}$ at (x,y') in $F_{x,y}$ identifies to the subspace of elements w of $[y',\mathfrak{g}]$ such that $\sigma'(x,y')(0,w)=0$. Hence, by Lemma 2.4(ii),

$$\mathrm{T}_{x,y'}(F_{x,y}) = [y',\mathfrak{g}] \cap V_{x,y'}^{\perp} = (\mathfrak{g}^{y'}+V_{x,y'})^{\perp},$$

since $[y',\mathfrak{g}] = (\mathfrak{g}^{y'})^{\perp}$. But by Lemma 2.3(ii), $(\mathfrak{g}^{y'}+V_{x,y'})^{\perp}$ has dimension at least $\frac{1}{2}\dim G.a$; so does $\mathrm{T}_{x,y'}(F_{x,y})$. This proves (i). Moreover, the equality holds if and only if $(\mathfrak{g}^{y'}+V_{x,y'})^{\perp}$ has dimension $\frac{1}{2}\dim G.a$, whence the statement (ii). □

THEOREM 2.7. *The following conditions are equivalent:*

(1) $\operatorname{ind}\mathfrak{g}^a = \ell$;
(2) π *has a fiber of dimension* $\frac{1}{2}\dim G.a$;
(3) *there exists* $(x,y)\in\mathfrak{g}\times G.a$ *such that* $(\mathfrak{g}^y+V_{x,y})^{\perp}$ *has dimension* $\frac{1}{2}\dim G.a$;
(4) *there exists* x *in* $\mathfrak{g}_{\mathrm{reg}}$ *such that* $\dim(\mathfrak{g}^a+V_{x,a}) = \frac{1}{2}(\dim\mathfrak{g}+\dim\mathfrak{g}^a)$;
(5) *there exists* x *in* $\mathfrak{g}_{\mathrm{reg}}$ *such that* $\dim V_{x,a} = \frac{1}{2}\dim G.a+\ell$;
(6) $\sigma(\mathfrak{g}\times\{a\})$ *has dimension* $\frac{1}{2}\dim G.a+\ell$.

Proof. By Theorem 1.1 and Remark 2.5, we have (1)⇔(2). Moreover, by Lemma 2.6(ii), we have (2)⇔(3).
(3)⇔(4): If (4) holds, so does (3). Indeed, if so,

$$\dim\mathfrak{g} - \frac{1}{2}\dim G.a = \frac{1}{2}(\dim\mathfrak{g}+\dim\mathfrak{g}^a) = \dim(\mathfrak{g}^a+V_{x,a}).$$

Conversely, suppose that (3) holds. By Lemma 2.3(ii), $\mathfrak{g}^y+V_{x,y}$ has maximal dimension $\frac{1}{2}(\dim\mathfrak{g}+\dim\mathfrak{g}^y)$. So the same goes for all (x,y) in a G-invariant nonempty open subset of $\mathfrak{g}\times G.a$. Hence, since the map $(x,y)\mapsto V_{x,y}$ is G-equivariant, there exists x in $\mathfrak{g}_{\mathrm{reg}}$ such that

$$\dim(V_{x,a}+\mathfrak{g}^a) = \frac{1}{2}(\dim\mathfrak{g}+\dim\mathfrak{g}^a).$$

(4)⇔(5): Let x be in $\mathfrak{g}_{\mathrm{reg}}$. By Lemma 2.3(iii), $[x,V_{x,a}]=[a,V_{x,a}]$. Hence $\mathfrak{g}^a\cap V_{x,a}$ has dimension ℓ by Remark 2.2(2). As a consequence,

$$\dim(\mathfrak{g}^a+V_{x,a}) = \dim\mathfrak{g}^a+\dim V_{x,a}-\ell,$$

whence the equivalence.

(2)⇔(6): Suppose that (2) holds. By Lemma 2.6, $\frac{1}{2}\dim G.a$ is the minimal dimension of the fibers of π. So, $\pi(\mathfrak{g}\times G.a)$ has dimension

$$\dim\mathfrak{g}+\dim G.a-\frac{1}{2}\dim G.a=\dim\mathfrak{g}+\frac{1}{2}\dim G.a.$$

Denote by τ the restriction to $\pi(\mathfrak{g}\times G.a)$ of the projection map $\mathfrak{g}\times \Bbbk^{\mathrm{b}_{\mathfrak{g}}+\ell}\rightarrow \Bbbk^{\mathrm{b}_{\mathfrak{g}}+\ell}$. Then $\tau\circ\pi$ is the restriction of σ to $\mathfrak{g}\times G.a$. Since σ is a G-invariant map, $\sigma(\mathfrak{g}\times\{a\})=\sigma(\mathfrak{g}\times G.a)$. Let $(x,y)\in\mathfrak{g}_{\mathrm{reg,ss}}\times G.a$. The fiber of τ at $z=\sigma(x,y)$ is $G.x$ since x is a regular semisimple element of $\mathfrak{g}$. Hence,

$$\dim\sigma(\mathfrak{g}\times\{a\}) \;=\; \dim\pi(\mathfrak{g}\times G.a)-(\dim\mathfrak{g}-\ell)=\frac{1}{2}\dim G.a+\ell$$

and we obtain (6).

Conversely, suppose that (6) holds. Then $\pi(\mathfrak{g}\times G.a)$ has dimension $\dim\mathfrak{g}+\frac{1}{2}\dim G.a$ by the above equality. So the minimal dimension of the fibers of π is equal to

$$\dim\mathfrak{g}+\dim G.a-(\dim\mathfrak{g}+\frac{1}{2}\dim G.a)=\frac{1}{2}\dim G.a$$

and (2) holds. □

2.3. Induced and rigid nilpotent orbits. The definitions and results of this subsection are mostly extracted from [Di74], [Di75], [LS79] and [BoK79]. We refer to [CMa93] and [TY05] for recent surveys.

Let $\mathfrak{p}$ be a proper parabolic subalgebra of $\mathfrak{g}$ and let $\mathfrak{l}$ be a reductive factor of $\mathfrak{p}$. We denote by $\mathfrak{p}_{\mathrm{u}}$ the nilpotent radical of $\mathfrak{p}$. Denote by L the connected closed subgroup of G whose Lie algebra is a$d\mathfrak{l}$ and denote by P the normalizer of $\mathfrak{p}$ in G.

Theorem 2.8 ([CMa93],Theorem 7.1.1). *Let $\mathcal{O}_{\mathfrak{l}}$ be a nilpotent orbit of $\mathfrak{l}$. There exists a unique nilpotent orbit $\mathcal{O}_{\mathfrak{g}}$ in $\mathfrak{g}$ whose intersection with $\mathcal{O}_{\mathfrak{l}}+\mathfrak{p}_{\mathrm{u}}$ is a dense open subset of $\mathcal{O}_{\mathfrak{l}}+\mathfrak{p}_{\mathrm{u}}$. Moreover, the intersection of $\mathcal{O}_{\mathfrak{g}}$ and $\mathcal{O}_{\mathfrak{l}}+\mathfrak{p}_{\mathrm{u}}$ consists of a single P-orbit and* $\mathrm{codim}_{\mathfrak{g}}(\mathcal{O}_{\mathfrak{g}})=\mathrm{codim}_{\mathfrak{l}}(\mathcal{O}_{\mathfrak{l}})$.

The orbit $\mathcal{O}_{\mathfrak{g}}$ only depends on $\mathfrak{l}$ and not on the choice of a parabolic subalgebra $\mathfrak{p}$ containing it [CMa93, Theorem 7.1.3]. By definition, the orbit $\mathcal{O}_{\mathfrak{g}}$ is called the *induced orbit from* $\mathcal{O}_{\mathfrak{l}}$; it is denoted by $\mathrm{Ind}_{\mathfrak{l}}^{\mathfrak{g}}(\mathcal{O}_{\mathfrak{l}})$. If $\mathcal{O}_{\mathfrak{l}}=0$, then we call $\mathcal{O}_{\mathfrak{g}}$ a *Richardson orbit.* For example all even nilpotent orbits are Richardson [CMa93, Corollary 7.1.7]. In turn, not all nilpotent orbits are induced from another one. A nilpotent orbit which is not induced in a proper way from another one is called *rigid.*

We shall say that $e\in\mathcal{N}(\mathfrak{g})$ is an induced (respectively rigid) nilpotent element of $\mathfrak{g}$ if the G-orbit of e is an induced (respectively rigid) nilpotent orbit of $\mathfrak{g}$. The following results are deeply linked to the properties of the sheets of $\mathfrak{g}$ and the deformations of its G-orbits. We refer to [BoK79] about these notions.

Theorem 2.9. (i) *Let x be a non nilpotent element of $\mathfrak{g}$ and let $\mathcal{O}_{\mathfrak{g}}$ be the induced nilpotent orbit from the adjoint orbit of x_n in $\mathfrak{g}^{x_s}$. Then $\mathcal{O}_{\mathfrak{g}}$ is the unique nilpotent orbit contained in $\overline{C(x)}$ whose dimension is $\dim G.x$. Furthermore, $\overline{C(x)} \cap \mathcal{N}(\mathfrak{g}) = \overline{\mathcal{O}_{\mathfrak{g}}}$ and $\overline{C(x)} \cap \mathcal{N}(\mathfrak{g})$ is the nullvariety in $\overline{C(x)}$ of f_i where i is an element of $\{1, \ldots, \ell\}$ such that $f_i(x) \neq 0$.*
(ii) *Conversely, if $\mathcal{O}_{\mathfrak{g}}$ is an induced nilpotent orbit, there exists a non nilpotent element x of $\mathfrak{g}$ such that $\overline{C(x)} \cap \mathcal{N}(\mathfrak{g}) = \overline{\mathcal{O}_{\mathfrak{g}}}$.*

Proof. (i) Let $\mathfrak{p}$ be a parabolic subalgebra of $\mathfrak{g}$ having $\mathfrak{g}^{x_s}$ as a Levi factor. Denote by $\mathfrak{p}_{\rm u}$ its nilpotent radical and by P the normalizer of $\mathfrak{p}$ in G. Let $\mathcal{O}'$ be the adjoint orbit of $x_{\rm n}$ in $\mathfrak{g}^{x_{\rm s}}$.

Claim 2.10. Let C be the P-invariant closed cone generated by x and let C_0 be the subset of nilpotent elements of C. Then $C = \Bbbk x_{\rm s} + \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$, $C_0 = \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$ and C_0 is an irreducible subset of dimension $\dim P(x)$.

Proof. The subset $x_{\rm s} + \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$ is an irreducible closed subset of $\mathfrak{p}$ containing $P(x)$. Moreover, its dimension is equal to

$$\dim \mathcal{O}' + \dim \mathfrak{p}_{\rm u} = \dim \mathfrak{g}^{x_{\rm s}} - \dim \mathfrak{g}^{x} + \dim \mathfrak{p}_{\rm u} = \dim \mathfrak{p} - \dim \mathfrak{g}^{x}.$$

Since the closure of $P(x)$ and $x_{\rm s} + \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$ are both irreducible subsets of $\mathfrak{g}$, they coincide. As a consequence, the set $\Bbbk x_{\rm s} + \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$ is contained in C. Since the former set is clearly a closed conical subset of $\mathfrak{g}$ containing x, $C = \Bbbk x_{\rm s} + \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$. Then we deduce that $C_0 = \overline{\mathcal{O}'} + \mathfrak{p}_{\rm u}$. □

Denote by $G \times_P \mathfrak{g}$ the quotient of $G \times \mathfrak{g}$ under the right action of P given by $(g, z).p := (gp, p^{-1}(z))$. The map $(g, z) \mapsto g(z)$ from $G \times \mathfrak{g}$ to $\mathfrak{g}$ factorizes through the quotient map from $G \times \mathfrak{g}$ to $G \times_P \mathfrak{g}$. Since G/P is a projective variety, the so obtained map from $G \times_P \mathfrak{g}$ to $\mathfrak{g}$ is closed. Since C and C_0 are closed P-invariant subsets of $\mathfrak{g}$, $G \times_P C$ and $G \times_P C_0$ are closed subsets of $G \times_P \mathfrak{g}$. Hence $\overline{C(x)} = G(C)$ and $G(C_0)$ is a closed subset of $\mathfrak{g}$. So, by the claim, the subset of nilpotent elements of $\overline{C(x)}$ is irreducible since C_0 is irreducible. Since there are finitely many nilpotent orbits, the subset of nilpotent elements of $\overline{C(x)}$ is the closure of one nilpotent orbit. Denote it by $\tilde{\mathcal{O}}$ and prove $\tilde{\mathcal{O}} = \mathcal{O}_{\mathfrak{g}}$.
For all k, l in $\{1, \ldots, \ell\}$, denote by $p_{k,l}$ the polynomial function

$$p_{k,l} := f_k(x)^{d_l} f_l^{d_k} - f_l(x)^{d_k} f_k^{d_l}$$

Then $p_{k,l}$ is G-invariant and homogeneous of degree $d_k d_l$. Moreover $p_{k,l}(x) = 0$. As a consequence, $\overline{C(x)}$ is contained in the nullvariety of

the functions $p_{k,l}$, $1 \leq k, l \leq \ell$. Hence the nullvariety of f_i in $\overline{C(x)}$ is contained in the nilpotent cone of $\mathfrak{g}$ since it is the nullvariety in $\mathfrak{g}$ of the functions $f_1, \dots, f_\ell$. Then $\dim \tilde{\mathcal{O}} = \dim \overline{C(x)} - 1 = \dim G.x$. Since $\mathcal{O}' + \mathfrak{p}_{\mathrm{u}}$ is contained in $\overline{C(x)}$, Theorem 2.8 tells us that $\mathcal{O}_{\mathfrak{g}}$ is contained in $\overline{C(x)}$. Moreover by Theorem 2.8, $\mathcal{O}_{\mathfrak{g}}$ has dimension $\dim G.x$, whence $\tilde{\mathcal{O}} = \mathcal{O}_{\mathfrak{g}}$. All statements of (i) are now clear.
(ii) By hypothesis, $\mathcal{O}_{\mathfrak{g}} = \mathrm{Ind}_{\mathfrak{l}}^{\mathfrak{g}}(\mathcal{O}_{\mathfrak{l}})$, where $\mathfrak{l}$ is a proper Levi subalgebra of $\mathfrak{g}$ and $\mathcal{O}_{\mathfrak{l}}$ a nilpotent orbit in $\mathfrak{l}$. Let x_{s} be an element of the center of $\mathfrak{l}$ such that $\mathfrak{g}^{x_{\mathrm{s}}} = \mathfrak{l}$, let x_{n} be an element of $\mathcal{O}_{\mathfrak{l}}$ and set $x = x_{\mathrm{s}} + x_{\mathrm{n}}$. Since $\mathfrak{l}$ is a proper subalgebra, the element x is not nilpotent. So by (i), the subset of nilpotent elements of $\overline{C(x)}$ is the closure of $\mathcal{O}_{\mathfrak{g}}$. □

3. Proof of Theorem 1.3 for induced nilpotent orbits

Let e be an induced nilpotent element. Let x be a non nilpotent element of $\mathfrak{g}$ such that $\overline{C(x)} \cap \mathcal{N}(\mathfrak{g}) = \overline{G.e}$. Such an element does exist by Theorem 2.9(ii).
As an abbreviation, we set:

$$\begin{aligned} \Bbbk^{\underline{d}} &:= \Bbbk^{d_1+1} \times \cdots \times \Bbbk^{d_\ell+1} \simeq \Bbbk^{\mathrm{b}_{\mathfrak{g}}+\ell}, \\ \Bbbk^{\underline{d}\times} &:= (\Bbbk^{d_1+1} \setminus \{0\}) \times \cdots \times (\Bbbk^{d_\ell+1} \setminus \{0\}), \\ \mathbb{P}^{\underline{d}} &:= \mathbb{P}(\Bbbk^{d_1+1}) \times \cdots \times \mathbb{P}(\Bbbk^{d_\ell+1}) = \mathbb{P}^{d_1} \times \cdots \times \mathbb{P}^{d_\ell}. \end{aligned}$$

For $j = 1, \dots, \ell$, recall that σ_j is the map:

$$\mathfrak{g} \times \mathfrak{g} \xrightarrow{\sigma_j} \Bbbk^{d_j+1}, \ (x, y) \mapsto (f_j^{(m)}(x, y))_{0 \leq m \leq d_j}.$$

Let $\mathcal{B}_j$ be the nullvariety of σ_j in $\mathfrak{g} \times \mathfrak{g}$ and let $\mathcal{B}$ be the union of $\mathcal{B}_1, \dots, \mathcal{B}_\ell$; it is a bicone of $\mathfrak{g} \times \mathfrak{g}$. Denote by ρ and τ the canonical maps:

$$\begin{array}{ccc} (\mathfrak{g} \times \mathfrak{g}) \setminus \{0\} & \xrightarrow{\rho} & \mathbb{P}(\mathfrak{g} \times \mathfrak{g}) \\ \Bbbk^{\mathrm{d}\times} & \xrightarrow{\tau} & \mathbb{P}^{\underline{d}}. \end{array}$$

Let σ^* be the restriction to $(\mathfrak{g} \times \mathfrak{g}) \setminus \mathcal{B}$ of σ; it has values in $\Bbbk^{\underline{d}\times}$. Since $\sigma_j(sx, sy) = s^{d_j} \sigma_j(x, y)$ for all $(x, y) \in \mathfrak{g} \times \mathfrak{g}$ and $j = 1, \dots, \ell$, the map $\tau \circ \sigma^*$ factors through ρ. Denote by $\overline{\sigma^*}$ the map from $\rho(\mathfrak{g} \times \mathfrak{g} \setminus \mathcal{B})$ to $\mathbb{P}^{\underline{d}}$ making the following diagram commutative:

$$\begin{array}{ccc} \mathfrak{g} \times \mathfrak{g} \setminus \mathcal{B} & \xrightarrow{\sigma^* = \sigma|_{\mathfrak{g} \times \mathfrak{g} \setminus \mathcal{B}}} & \Bbbk^{\underline{d}\times} \\ {\scriptstyle\rho}\downarrow & & \downarrow{\scriptstyle\tau} \\ \rho(\mathfrak{g} \times \mathfrak{g} \setminus \mathcal{B}) & \overset{\overline{\sigma^*}}{\dashrightarrow} & \mathbb{P}^{\underline{d}} \end{array}$$

and let Γ be the graph of the restriction to $\rho(\mathfrak{g} \times \overline{C(x)} \setminus \mathcal{B})$ of $\overline{\sigma^*}$.

Lemma 3.1. *The set* Γ *is a closed subset of* $\mathbb{P}(\mathfrak{g}\times\mathfrak{g})\times\mathbb{P}^{\underline{d}}$.

Proof. Let $\widetilde{\Gamma}$ be the inverse image of Γ by the map $\rho\times\tau$. Then $\widetilde{\Gamma}$ is the intersection of the graph of σ and $(\mathfrak{g}\times\overline{C(x)}\setminus\mathcal{B})\times\Bbbk^{\underline{d}\times}$. Since $\sigma^{-1}(\Bbbk^{\underline{d}}\setminus\Bbbk^{\underline{d}\times})$ is contained in $\mathcal{B}$, $\widetilde{\Gamma}$ is the intersection of the graph of σ and $(\mathfrak{g}\times\overline{C(x)}\setminus\{0\})\times\Bbbk^{\underline{d}\times}$; so $\widetilde{\Gamma}$ is closed in $(\mathfrak{g}\times\overline{C(x)})\setminus\{0\}\times\Bbbk^{\underline{d}\times}$. As a consequence, Γ is closed in $\mathbb{P}(\mathfrak{g}\times\mathfrak{g})\times\mathbb{P}^{\underline{d}}$, since $\mathbb{P}(\mathfrak{g}\times\mathfrak{g})\times\mathbb{P}^{\underline{d}}$ is endowed with the quotient topology. □

Denote by Z the closure of $\sigma(\mathfrak{g}\times\overline{C(x)})$ in $\Bbbk^{\underline{d}}$.

Lemma 3.2. *There exists an open subset* U *of* Z*, contained in* $\sigma(\mathfrak{g}\times\overline{C(x)})$*, such that* $U\cap\sigma(\mathfrak{g}\times G.e)$ *is not empty.*

Proof. Let Γ_2 be the projection of $\Gamma\subset\mathbb{P}(\mathfrak{g}\times\mathfrak{g})\times\mathbb{P}^{\underline{d}}$ to $\mathbb{P}^{\underline{d}}$. By Lemma 3.1, Γ_2 is a closed subset of $\mathbb{P}^{\underline{d}}$ since $\mathbb{P}(\mathfrak{g}\times\mathfrak{g})$ is complete. So $\tau^{-1}(\Gamma_2)$ is a closed subset of $\Bbbk^{\underline{d}\times}$. Moreover,

$$\tau^{-1}(\Gamma_2)=\sigma(\mathfrak{g}\times\overline{C(x)}\setminus\mathcal{B})$$

since $\sigma(\mathfrak{g}\times\overline{C(x)})$ is stable under the action of $\Bbbk^*\times\cdots\times\Bbbk^*$ on $\Bbbk^{\underline{d}}$. Hence the open subset $Z\cap\Bbbk^{\underline{d}\times}$ of Z is contained in $\sigma(\mathfrak{g}\times\overline{C(x)})$. But for all y in $\mathfrak{g}$ such that $f_j(y)\neq 0$ for any j, $\sigma(y,e)$ belongs to $\Bbbk^{\underline{d}\times}$. Thus, the open subset $U=Z\cap\Bbbk^{\underline{d}\times}$ of Z is convenient and the lemma follows. □

We are now ready to prove the main result of this section:

Theorem 3.3. *Assume that* $\operatorname{ind}\mathfrak{a}^x=\operatorname{rk}\mathfrak{a}$ *for all reductive subalgebras* $\mathfrak{a}$ *strictly contained in* $\mathfrak{g}$ *and for all* x *in* $\mathfrak{a}$*. Then for all induced nilpotent orbits* $\mathcal{O}_{\mathfrak{g}}$ *in* $\mathfrak{g}$ *and for all* e *in* $\mathcal{O}_{\mathfrak{g}}$*,* $\operatorname{ind}\mathfrak{g}^e=\ell$.

Proof. Let $\mathcal{O}_{\mathfrak{g}}$ be an induced nilpotent orbit and let e be in $\mathcal{O}_{\mathfrak{g}}$. Using Theorem 2.9(ii), we let x be a non nilpotent element of $\mathfrak{g}$ such that $\overline{C(x)}\cap\mathcal{N}(\mathfrak{g})=\overline{\mathcal{O}_{\mathfrak{g}}}$. Since x is not nilpotent, $\mathfrak{g}^x$ is the centralizer in the reductive Lie algebra $\mathfrak{g}^{x_{\rm s}}$ of the nilpotent element $x_{\rm n}$ of $\mathfrak{g}^{x_{\rm s}}$. Since $\mathfrak{g}^{x_{\rm s}}$ is strictly contained in $\mathfrak{g}$ and has rank ℓ, the index of $\mathfrak{g}^x$ is equal to ℓ by hypothesis. Besides, by Theorem 2.7, (1)⇒(6), applied to x,

$$\dim\sigma(\mathfrak{g}\times\{x\})=\frac{1}{2}\dim G.x+\ell.$$

Since σ is G-invariant, $\sigma(\mathfrak{g}\times\{x\})=\sigma(\mathfrak{g}\times G.x)$. Hence for all z in a dense subset of $\sigma(\mathfrak{g}\times G.x)$, the fiber of the restriction of σ to $\mathfrak{g}\times G.x$ at z has minimal dimension

$$\dim\mathfrak{g}+\dim G.x-(\frac{1}{2}\dim G.x+\ell)=\dim\mathfrak{g}+\frac{1}{2}\dim G.x-\ell.$$

Denote by Z the closure of $\sigma(\mathfrak{g}\times\overline{C(x)})$ in $\Bbbk^{\underline{d}}$. We deduce from the above equality that Z has dimension

$$\begin{aligned}\dim\mathfrak{g}+\dim C(x)-(\dim\mathfrak{g}+\frac{1}{2}\dim G.x-\ell) \\ &= \dim C(x)-\frac{1}{2}\dim G.x+\ell \\ &= \frac{1}{2}\dim G.e+\ell+1,\end{aligned}$$

since $\dim C(x)=\dim G.x+1=\dim G.e+1$.
By Lemma 3.2, there exists an open subset U of Z contained in $\sigma(\mathfrak{g}\times\overline{C(x)})$ having a nonempty intersection with $\sigma(\mathfrak{g}\times G.e)$. Let i be in $\{1,\dots,\ell\}$ such that $f_i(x)\neq 0$. For $z\in\Bbbk^{\underline{d}}$, we write $z=(z_{i,j})_{\substack{1\leq i\leq\ell\\ 0\leq j\leq d_i}}$ its coordinates. Let $\mathcal{V}_i$ be the nullvariety in U of the coordinate z_{i,d_i}. Then $\mathcal{V}_i$ is not empty by the choice of U. Since U is irreducible and since z_{i,d_i} is not identically zero on U, $\mathcal{V}_i$ is equidimensional of dimension $\frac{1}{2}\dim G.e+\ell$. By Theorem 2.9(i), the nullvariety of f_i in $\overline{C(x)}$ is equal to $\overline{G.e}$. Hence $\sigma^{-1}(\mathcal{V}_i)\cap(\mathfrak{g}\times\overline{C(x)})=\sigma^{-1}(U)\cap(\mathfrak{g}\times\overline{G.e})$ is an open subset of $\mathfrak{g}\times\overline{G.e}$. So $\sigma(\mathfrak{g}\times G.e)$ has dimension $\frac{1}{2}\dim G.e+\ell$. Then by Theorem 2.7, (6)⇒(1), the index of $\mathfrak{g}^e$ is equal to ℓ. □

From that point, our goal is to prove Theorem 1.3 for rigid nilpotent elements; Theorem 3.3 tells us that this is enough to complete the proof.

4. The Slodowy slice and the property (P)

In this section, we introduce a property (P) in Definition 4.2 and we prove that $e\in\mathcal{N}(\mathfrak{g})$ has Property (P) if and only if $\operatorname{ind}\mathfrak{g}^e=\ell$ (Theorem 4.13). Then, we will show in the next section that all rigid nilpotent orbits of $\mathfrak{g}$ but seven orbits (one in the type E_7 and six in the type E_8) do have Property (P).

4.1. Blowing up of $\mathcal{S}$. Let e be a nilpotent element of $\mathfrak{g}$ and consider an $\mathfrak{sl}_2$-triple (e,h,f) containing e as in Subsection 1.3. The *Slodowy slice* is the affine subspace $\mathcal{S}:=e+\mathfrak{g}^f$ of $\mathfrak{g}$ which is a transverse variety to the adjoint orbit $G.e$. Denote by $B_e(\mathcal{S})$ the blowing up of $\mathcal{S}$ centered at e and let $p: B_e(\mathcal{S})\to\mathcal{S}$ be the canonical morphism. The variety $\mathcal{S}$ is smooth and $p^{-1}(e)$ is a smooth irreducible hypersurface of $B_e(\mathcal{S})$. The use of the blowing-up $B_e(\mathcal{S})$ for the computation of the index was initiated by the first author in [Ch04] and resumed by the second author in [Mo06a]. Here, we use again this technique to study the index of $\mathfrak{g}^e$. Describe first the main tools extracted from [Ch04] we need.

For Y an open subset of $B_e(\mathcal{S})$, we denote by $\Bbbk[Y]$ the algebra of regular functions on Y. By [Ch04, Théorème 3.3], we have:

THEOREM 4.1. *The following two assertions are equivalent:*
(A) *the equality* $\operatorname{ind}\mathfrak{g}^e = \ell$ *holds,*
(B) *there exists an affine open subset* $Y \subset B_e(\mathcal{S})$ *such that* $Y \cap p^{-1}(e) \neq \emptyset$ *and satisfying the following property:*

> *for any regular map* $\varphi \in \Bbbk[Y] \otimes_{\Bbbk} \mathfrak{g}$ *such that* $\varphi(x) \in [\mathfrak{g}, p(x)]$ *for all* $x \in Y$*, there exists* $\psi \in \Bbbk[Y] \otimes_{\Bbbk} \mathfrak{g}$ *such that* $\varphi(x) = [\psi(x), p(x)]$ *for all* $x \in Y$*.*

An open subset $\Omega \subset B_e(\mathcal{S})$ is called *a big open subset* if $B_e(\mathcal{S}) \setminus \Omega$ has codimension at least 2 in $B_e(\mathcal{S})$. As explained in [Ch04, Section 2], there exists a big open subset Ω of $B_e(\mathcal{S})$ and a regular map

$$\alpha : \Omega \to \mathrm{Gr}_\ell(\mathfrak{g})$$

such that $\alpha(x) = \mathfrak{g}^{p(x)}$ if $p(x)$ is regular. Furthermore, the map α is uniquely defined by this condition. In fact, this result is a consequence of [Sh94, Ch. VI, Theorem 1]. From now on, α stands for the so-defined map. Since $p^{-1}(e)$ is an hypersurface and since Ω is a big open subset of $B_e(\mathcal{S})$, note that $\Omega \cap p^{-1}(e)$ is a nonempty set. In addition, $\alpha(x) \subset \mathfrak{g}^{p(x)}$ for all $x \in \Omega$.

DEFINITION 4.2. We say that e *has Property* (P) if $\mathfrak{z}(\mathfrak{g}^e) \subset \alpha(x)$ for all x in $\Omega \cap p^{-1}(e)$.

Remark 4.3. Suppose that e is regular. Then $\mathfrak{g}^e$ is a commutative algebra, i.e. $\mathfrak{z}(\mathfrak{g}^e) = \mathfrak{g}^e$. If $x \in \Omega \cap p^{-1}(e)$, then $\alpha(x) = \mathfrak{g}^e$ since $p(x) = e$ is regular in this case. On the other hand, $\operatorname{ind}\mathfrak{g}^e = \dim \mathfrak{g}^e = \ell$ since e is regular. So e has Property (P) and $\operatorname{ind}\mathfrak{g}^e = \ell$.

4.2. ON THE PROPERTY (P). This subsection aims to show: Property (P) holds for e if and only if $\operatorname{ind}\mathfrak{g}^e = \ell$. As a consequence of Remark 4.3, we can (and will) assume that e is a nonregular nilpotent element of $\mathfrak{g}$. As a first step, we will state in Corollary 4.12 that, if (P) holds, then so does the assertion (B) of Theorem 4.1.
Let $L_{\mathfrak{g}}$ be the $\mathrm{S}(\mathfrak{g})$-submodule of $\varphi \in \mathrm{S}(\mathfrak{g}) \otimes_{\Bbbk} \mathfrak{g}$ satisfying $[\varphi(x), x] = 0$ for all x in $\mathfrak{g}$. It is known that $L_{\mathfrak{g}}$ is a free module of basis $\varphi_1, \ldots, \varphi_\ell$, cf. [Di79]. We investigate an analogous property for the Slodowy slice $\mathcal{S} = e + \mathfrak{g}^f$. We denote by $\mathcal{S}_{\mathrm{reg}}$ the intersection of $\mathcal{S}$ and $\mathfrak{g}_{\mathrm{reg}}$. As e is nonregular, the set $(\mathcal{S} \setminus \mathcal{S}_{\mathrm{reg}})$ contains e.

LEMMA 4.4. *The set* $\mathcal{S} \setminus \mathcal{S}_{\mathrm{reg}}$ *has codimension* 3 *in* $\mathcal{S}$ *and each irreducible component of* $\mathcal{S} \setminus \mathcal{S}_{\mathrm{reg}}$ *contains* e.

Proof. Let us consider the morphism

$$\begin{array}{ccc} G \times \mathcal{S} & \longrightarrow & \mathfrak{g} \\ (g,x) & \longmapsto & g(x) \end{array}$$

By a Slodowy's result [Sl80], this morphism is a smooth morphism. So its fibers are equidimensional of dimension $\dim \mathfrak{g}^f$. In addition, by [V72], $\mathfrak{g}\setminus\mathfrak{g}_{\rm reg}$ is a G-invariant equidimensional closed subset of $\mathfrak{g}$ of codimension 3. Hence $\mathcal{S}\setminus\mathcal{S}_{\rm reg}$ is an equidimensional closed subset of $\mathcal{S}$ of codimension 3.

Denoting by $t \mapsto g(t)$ the one parameter subgroup of G generated by ad$h$, $\mathcal{S}$ and $\mathcal{S}\setminus\mathcal{S}_{\rm reg}$ are stable under the action of $t^{-2}g(t)$ for all t in $\Bbbk^*$. Furthermore, for all x in $\mathcal{S}$, $t^{-2}g(t)(x)$ goes to e when t goes to ∞, whence the lemma. □

Denote by $\Bbbk[\mathcal{S}]$ the algebra of regular functions on $\mathcal{S}$ and denote by $L_{\mathcal{S}}$ the $\Bbbk[\mathcal{S}]$-submodule of $\varphi \in \Bbbk[\mathcal{S}]\otimes_{\Bbbk}\mathfrak{g}$ satisfying $[\varphi(x),x]=0$ for all x in $\mathcal{S}$.

Lemma 4.5. *The module $L_{\mathcal{S}}$ is a free module of basis $\varphi_1|_{\mathcal{S}},\ldots,\varphi_\ell|_{\mathcal{S}}$ where $\varphi_i|_{\mathcal{S}}$ is the restriction to $\mathcal{S}$ of φ_i for $i=1,\ldots,\ell$.*

Proof. Let φ be in $L_{\mathcal{S}}$. There are regular functions $a_1,\ldots,a_\ell$ on $\mathcal{S}_{\rm reg}$ satisfying

$$\varphi(x) = a_1(x)\varphi_1|_{\mathcal{S}}(x) + \cdots + a_\ell(x)\varphi_\ell|_{\mathcal{S}}(x)$$

for all $x\in\mathcal{S}_{\rm reg}$, by Lemma 2.1(ii). By Lemma 4.4, $\mathcal{S}\setminus\mathcal{S}_{\rm reg}$ has codimension 3 in $\mathcal{S}$. Hence $a_1,\ldots,a_\ell$ have polynomial extensions to $\mathcal{S}$ since $\mathcal{S}$ is normal. So the maps $\varphi_1|_{\mathcal{S}},\ldots,\varphi_\ell|_{\mathcal{S}}$ generate $L_{\mathcal{S}}$. Moreover, by Lemma 2.1(ii) for all $x\in\mathcal{S}_{\rm reg}$, $\varphi_1(x),\ldots,\varphi_\ell(x)$ are linearly independent, whence the statement. □

The following proposition accounts for an important step to interpret Assertion (B) of Theorem 4.1:

Proposition 4.6. *Let φ be in $\Bbbk[\mathcal{S}]\otimes_{\Bbbk}\mathfrak{g}$ such that $\varphi(x)\in[\mathfrak{g},x]$ for all x in a nonempty open subset of $\mathfrak{g}$. Then there exists a polynomial map $\psi\in\Bbbk[\mathcal{S}]\otimes_{\Bbbk}\mathfrak{g}$ such that $\varphi(x)=[\psi(x),x]$ for all $x\in\mathcal{S}$.*

Proof. Since $\mathfrak{g}^x$ is the orthogonal complement of $[x,\mathfrak{g}]$ in $\mathfrak{g}$, our hypothesis says that $\varphi(x)$ is orthogonal to $\mathfrak{g}^x$ for all x in a nonempty open subset $\mathcal{S}'$ of $\mathcal{S}$. The intersection $\mathcal{S}'\cap\mathcal{S}_{\rm reg}$ is not empty; so by Lemma 2.1(ii), $\langle\varphi(x),\varphi_i|_{\mathcal{S}}(x)\rangle=0$ for all $i=1,\ldots,\ell$ and for all $x\in\mathcal{S}'\cap\mathcal{S}_{\rm reg}$. Therefore, by continuity, $\langle\varphi(x),\varphi_i|_{\mathcal{S}}(x)\rangle=0$ for all $i=1,\ldots,\ell$ and all $x\in\mathcal{S}$. Hence $\varphi(x)\in[x,\mathfrak{g}]$ for all $x\in\mathcal{S}_{\rm reg}$ by Lemma 2.1(ii) again. Consequently by Lemma 4.4, Lemma 4.5 and the proof of the main theorem of [Di79], there exists an element $\psi \in \Bbbk[\mathcal{S}] \otimes_{\Bbbk} \mathfrak{g}$ which satisfies the condition of the proposition. $\square$

Let $u_1,\ldots,u_m$ be a basis of $\mathfrak{g}^f$ and let $u_1^*,\ldots,u_m^*$ be the corresponding coordinate system of $\mathcal{S} = e + \mathfrak{g}^f$. There is an affine open subset $Y \subset B_e(\mathcal{S})$ with $Y \cap p^{-1}(e) \neq \emptyset$ such that $\Bbbk[Y]$ is the set of linear combinations of monomials in $(u_1^*)^{-1}, u_1^*,\ldots,u_m^*$ whose total degree is nonnegative. In particular, we have a global coordinates system $u_1^*, v_2^*,\ldots,v_m^*$ on Y satisfying the relations:

$$u_2^* = u_1^* v_2^* \quad ,\ldots, \quad u_m^* = u_1^* v_m^*. \tag{4}$$

Note that, for $x \in Y$, we so have: $p(x) = e + u_1^*(x)(u_1 + v_2^*(x)u_2 + \cdots + v_m^*(x)u_m)$. So, the image of Y by p is the union of $\{e\}$ and the complementary in $\mathcal{S}$ of the nullvariety of u_1^*. Let Y' be an affine open subset of Y contained in Ω and having a nonempty intersection with $p^{-1}(e)$. Denote by $L_{Y'}$ the set of regular maps φ from Y' to $\mathfrak{g}$ satisfying $[\varphi(x), p(x)] = 0$ for all $x \in Y'$.

Lemma 4.7. *Suppose that e has Property* (P). *For each $z \in \mathfrak{z}(\mathfrak{g}^e)$, there exists $\psi_z \in \Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $z - u_1^*\psi_z$ belongs to $L_{Y'}$.*

Proof. Let z be in $\mathfrak{z}(\mathfrak{g}^e)$. Since $Y' \subset \Omega$, for each $y \in Y'$, there exists an affine open subset U_y of Y' containing y and regular maps $\nu_1,\ldots,\nu_\ell$ from U_y to $\mathfrak{g}$ such that $\nu_1(x),\ldots,\nu_\ell(x)$ is a basis of $\alpha(x)$ for all $x \in U_y$. Let y be in Y'. We consider two cases:
(1) Suppose $p(y) = e$.
Since e has Property (P), there exist regular functions $a_1,\ldots,a_\ell$ on U_y satisfying

$$z = a_1(x)\nu_1(x) + \cdots + a_\ell(x)\nu_\ell(x),$$

for all $x \in U_y \cap p^{-1}(e)$. The intersection $U_y \cap p^{-1}(e)$ is the set of zeroes of u_1^* in U_y. So there exists a regular map ψ from U_y to $\mathfrak{g}$ which satisfies the equality:

$$z - u_1^*\psi = a_1\nu_1 + \cdots + a_\ell\nu_\ell.$$

Hence $[z - u_1^*(x)\psi(x), p(x)] = 0$ for all $x \in U_y$ since $\alpha(x)$ is contained in $\mathfrak{g}^{p(x)}$ for all $x \in \Omega$.
(2) Suppose $p(y) \neq e$.
Then we can assume that $U_y \cap p^{-1}(e) = \emptyset$ and the map $\psi = (u_1^*)^{-1}z$ satisfies the condition: $[z - u_1^*(x)\psi(x), p(x)] = 0$ for all $x \in U_y$.
In both cases (1) or (2), we have found a regular map ψ_y from U_y to $\mathfrak{g}$ satisfying: $[z - (u_1^*\psi_y)(x), p(x)] = 0$ for all $x \in U_y$.
Let $y_1,\ldots,y_k$ be in Y' such that the open subsets $U_{y_1},\ldots,U_{y_k}$ cover Y'. For $i = 1,\ldots,k$, we denote by ψ_i a regular map from U_{y_i} to $\mathfrak{g}$ such that $z - u_1^*\psi_i$ is in $\Gamma(U_{y_i}, \mathcal{L})$ where $\mathcal{L}$ is the localization of $L_{Y'}$ on Y'.

Then for $i, j = 1, \dots, k$, $\psi_i - \psi_j$ is in $\Gamma(U_{y_i} \cap U_{y_j}, \mathcal{L})$. Since Y' is affine, $\mathrm{H}^1(Y', \mathcal{L}) = 0$. So, for $i = 1, \dots, l$, there exists $\widetilde{\psi}_i$ in $\Gamma(U_{y_i}, \mathcal{L})$ such that $\widetilde{\psi}_i - \widetilde{\psi}_j$ is equal to $\psi_i - \psi_j$ on $U_{y_i} \cap U_{y_j}$ for all i, j. Then there exists a well-defined map ψ_z from Y' to $\mathfrak{g}$ whose restriction to U_{y_i} is equal to $\psi_i - \widetilde{\psi}_i$ for all i, and such that $z - u_1^* \psi_z$ belongs to $L_{Y'}$. Finally, the map ψ_z verifies the required property. □

Let z be in $\mathfrak{z}(\mathfrak{g}^e)$. We denote by φ_z the regular map from Y to $\mathfrak{g}$ defined by:

$$\varphi_z(x) = [z, u_1] + v_2^*(x)[z, u_2] + \cdots + v_m^*(x)[z, u_m], \quad \text{for all } x \in Y. \tag{5}$$

Corollary 4.8. *Suppose that e has Property* (P) *and let z be in $\mathfrak{z}(\mathfrak{g}^e)$. There exists ψ_z in $\Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $\varphi_z(x) = [\psi_z(x), p(x)]$ for all $x \in Y'$.*

Proof. By Lemma 4.7, there exists ψ_z in $\Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $z - u_1^* \psi_z$ is in $L_{Y'}$. Then

$$u_1^* \varphi_z(x) = [z, p(x)] = [z - u_1^* \psi_z(x), p(x)] + u_1^*[\psi_z(x), p(x)],$$

for all $x \in Y'$. So the map ψ_z is convenient, since u_1^* is not identically zero on Y'. □

The following lemma is easy but helpful for Proposition 4.10:

Lemma 4.9. *Let v be in $\mathfrak{g}^e$. Then, v belongs to $\mathfrak{z}(\mathfrak{g}^e)$ if and only if $[v, \mathfrak{g}^f] \subset [e, \mathfrak{g}]$.*

Proof. Since $[x, \mathfrak{g}]$ is the orthogonal complement of $\mathfrak{g}^x$ in $\mathfrak{g}$ for all $x \in \mathfrak{g}$, we have:

$$[v, \mathfrak{g}^f] \subset [e, \mathfrak{g}] \iff \langle [v, \mathfrak{g}^f], \mathfrak{g}^e \rangle = 0$$
$$\iff \langle [v, \mathfrak{g}^e], \mathfrak{g}^f \rangle = 0 \iff [v, \mathfrak{g}^e] \subset [f, \mathfrak{g}].$$

But $\mathfrak{g}$ is the direct sum of $\mathfrak{g}^e$ and $[f, \mathfrak{g}]$ and $[v, \mathfrak{g}^e]$ is contained in $\mathfrak{g}^e$ since $v \in \mathfrak{g}^e$. Hence $[v, \mathfrak{g}^f]$ is contained in $[e, \mathfrak{g}]$ if and only if v is in $\mathfrak{z}(\mathfrak{g}^e)$. □

Proposition 4.10. *Suppose that e has Property* (P) *and let φ be in $\Bbbk[Y] \otimes_{\Bbbk} \mathfrak{g}$ such that $\varphi(x) \in [\mathfrak{g}, p(x)]$ for all $x \in Y$. Then there exists ψ in $\Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $\varphi(x) = [\psi(x), p(x)]$ for all $x \in Y'$.*

Proof. Since φ is a regular map from Y to $\mathfrak{g}$, there is a nonnegative integer d and $\widetilde{\varphi} \in \Bbbk[\mathcal{S}] \otimes_{\Bbbk} \mathfrak{g}$ such that

$$(u_1^*)^d(x)\varphi(x) = (\widetilde{\varphi} \circ p)(x), \ \forall x \in Y \tag{6}$$

and $\widetilde{\varphi}$ is a linear combination of monomials in $u_1^*, \dots, u_m^*$ whose total degree is at least d. By hypothesis on φ, we deduce that for all $x \in \mathcal{S}$

such that $u_1^*(x) \neq 0$, $\widetilde{\varphi}(x)$ is in $[\mathfrak{g}, x]$. Hence by Proposition 4.6, there exists $\widetilde{\psi}$ in $\Bbbk[\mathcal{S}] \otimes_k \mathfrak{g}$ such that $\widetilde{\varphi}(x) = [\widetilde{\psi}(x), x]$ for all $x \in \mathcal{S}$.
Denote by $\widetilde{\psi}'$ the sum of monomials of degree at least d in $\widetilde{\psi}$ and denote by ψ' the element of $\Bbbk[Y] \otimes_{\Bbbk} \mathfrak{g}$ satisfying

$$(7) \qquad (u_1^*)^d(x)\psi'(x) = (\widetilde{\psi}'\circ p)(x), \ \forall x \in Y.$$

Then we set, for $x \in Y$, $\varphi'(x) := \varphi(x) - [\psi'(x), p(x)]$. We have to prove the existence of an element ψ'' in $\Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $\varphi'(x) = [\psi''(x), p(x)]$ for all $x \in Y'$.

• If $d = 0$, then $\varphi = \widetilde{\varphi}\circ p$, $\psi' = \psi$ and $\varphi' = 0$; so ψ' is convenient in that case.

• If $d = 1$, we can write

$$\begin{aligned} u_1^*(x)\varphi(x) &= \widetilde{\varphi}(p(x)) \\ &= [\widetilde{\psi}(p(x)), e + u_1^*(x)(u_1 + v_2^*(x)u_2 + \cdots + v_m^*(x)u_m)], \end{aligned}$$

for all $x \in Y$, whence we deduce

$$\begin{aligned} &u_1^*(x)(\varphi(x) - [\psi'(x), p(x)]) \\ &\qquad = [\tilde{\psi}(e), e + u_1^*(x)(u_1 + v_2^*(x)u_2 + \cdots + v_m^*(x)u_m)] \end{aligned}$$

for all $x \in Y$. Hence $\tilde{\psi}(e)$ belongs to $\mathfrak{g}^e$ and $[\widetilde{\psi}(e), u_i] \in [e, \mathfrak{g}]$ for all $i = 1, \ldots, m$, since $\varphi(x) \in [e, \mathfrak{g}]$ for all $x \in Y \cap p^{-1}(e)$. Then $\widetilde{\psi}(e)$ is in $\mathfrak{z}(\mathfrak{g}^e)$ by Lemma 4.9. So by Corollary 4.8, φ' has the desired property.

• Suppose $d > 1$. For $\underline{i} = (i_1, \ldots, i_m) \in \mathbb{N}^m$, we set $|\underline{i}| := i_1 + \cdots + i_m$ and we denote by $\psi_{\underline{i}}$ the coefficient of $(u_1^*)^{i_1} \cdots (u_m^*)^{i_m}$ in $\widetilde{\psi}$. By Corollary 4.8, it suffices to prove:

$$\begin{cases} \psi_{\underline{i}} = 0 & \text{if } |\underline{i}| < d-1; \\ \psi_{\underline{i}} \in \mathfrak{z}(\mathfrak{g}^e) & \text{if } |\underline{i}| = d-1 \end{cases}.$$

For $\underline{i} \in \mathbb{N}^m$ and $j \in \{1, \ldots, m\}$, we define the element $\underline{i}(j)$ of $\mathbb{N}^m$ by:

$$i(j) := (i_1, \ldots, i_{j-1}, i_j + 1, i_{j+1}, \ldots, i_m).$$

It suffices to prove:

Claim 4.11. For $|i| \leq d-1$, $\psi_{\underline{i}}$ is an element of $\mathfrak{g}^e$ such that $[\psi_{\underline{i}}, u_j] + [\psi_{\underline{i}(j)}, e] = 0$ for $j = 1, \ldots, m$.

Indeed, by Lemma 4.9, if

$$[\psi_{\underline{i}}, u_j] + [\psi_{\underline{i}(j)}, e] = 0 \text{ and } \psi_{\underline{i}} \in \mathfrak{g}^e$$

for all $j = 1, \ldots, m$, then $\psi_{\underline{i}} \in \mathfrak{z}(\mathfrak{g}^e)$. Furthermore, if

$$[\psi_{\underline{i}}, u_j] + [\psi_{\underline{i}(j)}, e] = 0 \text{ and } \psi_{\underline{i}} \in \mathfrak{g}^e \text{ and } \psi_{\underline{i}(j)} \in \mathfrak{g}^e$$

for all $j = 1, \ldots, m$, then $\psi_{\underline{i}} = 0$ since $\mathfrak{z}(\mathfrak{g}^e) \cap \mathfrak{g}^f = 0$. So only remains to prove Claim 4.11.

We prove the claim by induction on $|\underline{i}|$. Arguing as in the case $d = 1$, we prove the claim for $|\underline{i}| = 0$. We suppose the claim true for all $|\underline{i}| \leq l - 1$ for some $0 < l \leq d - 2$. We have to prove the statement for all $|i| \leq l$. By what foregoes and by induction hypothesis, $\psi_{\underline{i}} = 0$ for $|\underline{i}| \leq l - 2$. For $k = l+1, l+2$, we consider the ring $\Bbbk[\tau_k]$ where $\tau_k^k = 0$. Since $(u_1^*)^d$ vanishes on the set of $\Bbbk[\tau_{l+1}]$-points $x = x_0 + x_1\tau_{l+1} + \cdots + x_l\tau_{l+1}^l$ of Y whose source x_0 is a zero of u_1^*,

$$0 = [\widetilde{\psi}(e + \tau_{l+1}v), e + \tau_{l+1}v] = \sum_{|i|=l} \tau_{l+1}^l [\psi_{\underline{i}}, e](u_1^*)^{i_1} \cdots (u_m^*)^{i_m}(v),$$

for all $v \in \mathfrak{g}^f$. So $\psi_{\underline{i}} \in \mathfrak{g}^e$ for $|\underline{i}| = l$.

For $|\underline{i}|$ equal to l, the term in

$$\tau_{l+2}^{l+1}(u_1^*)^{i_1} \cdots (u_{i_{j-1}}^*)^{i_{j-1}}(u_{i_j+1}^*)^{i_j+1}(u_{i_{j+1}}^*)^{i_{j+1}} \cdots (u_m^*)^{i_m}(v)$$

of $[\widetilde{\psi}(e + \tau_{l+2}v), e + \tau_{l+2}v]$ is equal to $[\psi_{\underline{i}(j)}, e] + [\psi_{\underline{i}}, u_j]$. Since $(u_1^*)^d$ vanishes on the set of $\Bbbk[\tau_{l+2}]$-points of Y whose source is a zero of u_1^*, this term is equal to 0, whence the claim. □

Recall that Y' is an affine open subset of Y contained in Ω and having a nonempty intersection with $p^{-1}(e)$.

Corollary 4.12. *Suppose that e has Property* (P). *Let φ be in $\Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $\varphi(x) \in [\mathfrak{g}, p(x)]$ for all $x \in Y'$. Then there exists ψ in $\Bbbk[Y'] \otimes_{\Bbbk} \mathfrak{g}$ such that $\varphi(x) = [\psi(x), p(x)]$ for all $x \in Y'$.*

Proof. For $a \in \Bbbk[Y]$, denote by $D(a)$ the principal open subset defined by a. Let $D(a_1), \ldots, D(a_m)$ be an open covering of Y' by principal open subsets of Y, with $a_1, \ldots, a_k$ in $\Bbbk[Y]$. Since φ is a regular map from Y' to $\mathfrak{g}$, there is $m_i \geq 0$ such that $a_i^{m_i}\varphi$ is the restriction to Y' of some regular map φ_i from Y to $\mathfrak{g}$. For m_i big enough, φ_i vanishes on $Y \setminus D(a_i)$; hence $\varphi_i(x) \in [\mathfrak{g}, p(x)]$ for all $x \in Y$. So, by Proposition 4.6, there is a regular map ψ_i from Y' to $\mathfrak{g}$ such that $\varphi_i(x) = [\psi_i(x), p(x)]$ for all $x \in Y'$. Then for all $x \in D(a_i)$, we have $\varphi(x) = [a_i(x)^{-m_i}\psi_i(x), p(x)]$. Since Y' is an affine open subset of Y, there exists a regular map ψ from Y' to $\mathfrak{g}$ which satisfies the condition of the corollary. □

We are now in position to prove the main result of this section:

Theorem 4.13. *The equality* $\operatorname{ind} \mathfrak{g}^e = \ell$ *holds if and only if e has Property* (P).

Proof. By Corollary 4.12, if e has Property (P), then Assertion (B) of Theorem 4.1 is satisfied. Conversely, suppose that $\operatorname{ind}\mathfrak{g}^e = \ell$ and show that e has Property (P). By Theorem 4.1, (A)⇒(B), Assertion (B) is satisfied. We choose an affine open subset Y' of Y, contained in Ω, such that $Y' \cap p^{-1}(e) \neq$ and verifying the condition of the assertion (B). Let $z \in \mathfrak{z}(\mathfrak{g}^e)$. Recall that the map φ_z is defined by (5). Let x be in Y'. If $u_1^*(x) \neq 0$, then $\varphi_z(x)$ belongs to $[\mathfrak{g}, p(x)]$ by (5). If $u_1^*(x) = 0$, then by Lemma 4.9, $\varphi_z(x)$ belongs to $[e, \mathfrak{g}]$. So there exists a regular map ψ from Y' to $\mathfrak{g}$ such that $\varphi_z(x) = [\psi(x), p(x)]$ for all $x \in Y'$ by Assertion (B). Hence we have

$$[z - u_1^*\psi(x), p(x)] = 0,$$

for all $x \in Y'$ since $(u_1^*\varphi_z)(x) = [z, p(x)]$ for all $x \in Y$. So $\alpha(x)$ contains z for all x in $\Omega \cap Y' \cap p^{-1}(e)$. Since $p^{-1}(e)$ is irreducible, we deduce that e has Property (P). □

4.3. A new formulation of the property (P). Recall that Property (P) is introduced in Definition 4.2. As has been noticed in the proof of Lemma 4.4, the morphism $G \times \mathcal{S} \to \mathfrak{g}, (g, x) \mapsto g(x)$ is smooth. As a consequence, the set $\mathcal{S}_{\rm reg}$ of $v \in \mathcal{S}$ such that v is regular is a nonempty open subset of $\mathcal{S}$. For x in $\mathcal{S}_{\rm reg}$, $\mathfrak{g}^{e+t(x-e)}$ has dimension ℓ for all t in a nonempty open subset of $\Bbbk$ since $x = e + (x - e)$ is regular. Furthermore, since $\Bbbk$ has dimension 1, [Sh94, Ch. VI, Theorem 1] asserts that there is a unique regular map

$$\beta_x : \Bbbk \to \mathrm{Gr}_\ell(\mathfrak{g})$$

satisfying $\beta_x(t) = \mathfrak{g}^{e+t(x-e)}$ for all t in a nonempty open subset of $\Bbbk$. Recall that Y is an affine open subset of $B_e(\mathcal{S})$ with $Y \cap p^{-1}(e) \neq \emptyset$ and that $u_1^*, v_2^*, \ldots, v_m^*$ is a global coordinates system of Y, cf. (4). Let $\mathcal{S}'_{\rm reg}$ be the subset of x in $\mathcal{S}_{\rm reg}$ such that $u_1^*(x) \neq 0$. For x in $\mathcal{S}'_{\rm reg}$, we denote by $\widetilde{x}$ the element of Y whose coordinates are $0, v_2^*(x), \ldots, v_m^*(x)$.

Lemma 4.14. *Let x be in $\mathcal{S}'_{\rm reg}$.*
(i) *The subspace $\beta_x(0)$ is contained in $\mathfrak{g}^e$.*
(ii) *If $\widetilde{x} \in \Omega$, then $\alpha(\widetilde{x}) = \beta_x(0)$.*

Proof. (i) The map β_x is a regular map and $[\beta_x(t), e + t(x - e)] = 0$ for all t in a nonempty open subset of $\Bbbk$. So, $\beta_x(0)$ is contained in $\mathfrak{g}^e$.
(ii) Since $\mathcal{S}'_{\rm reg}$ has an empty intersection with the nullvariety of u_1^* in $\mathcal{S}$, the restriction of p to $p^{-1}(\mathcal{S}'_{\rm reg})$ is an isomorphism from $p^{-1}(\mathcal{S}'_{\rm reg})$ to $\mathcal{S}'_{\rm reg}$. Furthermore, $\beta_x(t) = \alpha(p^{-1}(e + tx - te))$ for any t in $\Bbbk$ such that $e + t(x - e)$ belongs to $\mathcal{S}'_{\rm reg}$ and $p^{-1}(e + tx - te)$ goes to $\widetilde{x}$ when t goes to 0. Hence $\beta_x(0)$ is equal to $\alpha(\widetilde{x})$ since α and β are regular maps. □

COROLLARY 4.15. *The element e has Property* (P) *if and only if* $\mathfrak{z}(\mathfrak{g}^e) \subset \beta_x(0)$ *for all x in a nonempty open subset of* $\mathcal{S}_{\rm reg}$.

Proof. The map $x \mapsto \widetilde{x}$ from $\mathcal{S}'_{\rm reg}$ to Y is well-defined and its image is an open subset of $Y \cap p^{-1}(e)$. Let $\mathcal{S}''_{\rm reg}$ be the set of $x \in \mathcal{S}'_{\rm reg}$ such that $\widetilde{x} \in \Omega$ and let Y'' be the image of $\mathcal{S}''_{\rm reg}$ by the map $x \mapsto \widetilde{x}$. Then $\mathcal{S}''_{\rm reg}$ is open in $\mathcal{S}_{\rm reg}$ and Y'' is dense in $\Omega \cap p^{-1}(e)$ since $p^{-1}(e)$ is irreducible. Furthermore, the image of a dense open subset of $\mathcal{S}''_{\rm reg}$ by the map $x \mapsto \widetilde{x}$ is dense in Y''. Since α is regular, e has property (P) if and only if $\alpha(x)$ contains $\mathfrak{z}(\mathfrak{g}^e)$ for all x in a dense subset of Y''. By Lemma 4.14(ii), the latter property is equivalent to the fact that $\beta_x(0)$ contains $\mathfrak{z}(\mathfrak{g}^e)$ for all x in a dense open subset of $\mathcal{S}''_{\rm reg}$. □

COROLLARY 4.16. (i) *If $\mathfrak{z}(\mathfrak{g}^e)$ is generated by $\varphi_1(e), \ldots, \varphi_\ell(e)$, then e has Property* (P).
(ii) *If $\mathfrak{z}(\mathfrak{g}^e)$ has dimension 1, then e has Property* (P).

Proof. Recall that $\varphi_i(e)$ belongs to $\mathfrak{z}(\mathfrak{g}^e)$, for all $i = 1, \ldots, \ell$, by Lemma 2.1(i). Moreover, for all x in $\mathcal{S}_{\rm reg}$ and all $i = 1, \ldots, \ell$, $\varphi_i(e + t(x - e))$ belongs to $\mathfrak{g}^{e+t(x-e)}$ for any t in $\Bbbk$. So by continuity, $\varphi_i(e)$ belongs to $\beta_x(0)$. As a consequence, whenever $\mathfrak{z}(\mathfrak{g}^e)$ is generated by $\varphi_1(e), \ldots, \varphi_\ell(e)$, e has Property (P) by Corollary 4.15.
(ii) is an immediate consequence of (i) since $\varphi_1(e) = e$ by our choice of d_1. □

5. PROOF OF THEOREM 1.3 FOR RIGID NILPOTENT ORBITS

We intend to prove in this section the following theorem:

THEOREM 5.1. *Suppose that $\mathfrak{g}$ is reductive and let e be a rigid nilpotent element of $\mathfrak{g}$. Then the index of $\mathfrak{g}^e$ is equal to ℓ.*

Theorem 5.1 will complete the proof of Theorem 1.3 by Theorem 3.3. As explained in introduction, we can assume that $\mathfrak{g}$ is simple. We consider two cases, according to $\mathfrak{g}$ has classical type or exceptional type.

5.1. THE CLASSICAL CASE. Assume that $\mathfrak{g}$ is simple of classical type. More precisely, assume that $\mathfrak{g}$ is one of the Lie algebras $\mathfrak{sl}_{\ell+1}(\Bbbk)$, $\mathfrak{so}_{2\ell+1}(\Bbbk)$, $\mathfrak{sp}_{2\ell}(\Bbbk)$, $\mathfrak{so}_{2\ell}(\Bbbk)$.

LEMMA 5.2. *Let m be a positive integer such that $x^m - \operatorname{tr} x^m$ belongs to $\mathfrak{g}$ for all x in $\mathfrak{g}$. Then e^m belongs to the subspace generated by $\varphi_1(e), \ldots, \varphi_\ell(e)$.*

Proof. Recall that $L_\mathfrak{g}$ is the submodule of elements φ of $\mathrm{S}(\mathfrak{g}) \otimes_\Bbbk \mathfrak{g}$ such that $[x, \varphi(x)] = 0$ for all x in $\mathfrak{g}$. According to [Di79], $L_\mathfrak{g}$ is a free module generated by the $\varphi_i's$. For all x in $\mathfrak{g}$, $[x,x^m]=0$. Hence there exist polynomial functions $a_1,\dots,a_\ell$ on $\mathfrak{g}$ such that

$$x^m - \operatorname{tr} x^m = a_1(x)\varphi_1(x)+\cdots+a_\ell(x)\varphi_\ell(x)$$

for all x in $\mathfrak{g}$, whence the lemma. □

Theorem 5.3. *Let e be a rigid nilpotent element. Then $\mathfrak{z}(\mathfrak{g}^e)$ is generated by powers of e. In particular, the index of $\mathfrak{g}^e$ is equal to ℓ.*

Proof. Let us prove the first assertion. If $\mathfrak{g}$ has type A or C, then $\mathfrak{z}(\mathfrak{g}^e)$ is generated by powers of e by [Mo06c, Théorème 1.1.8] or [Y06b]. So we can assume that $\mathfrak{g}$ has type B or D.
Set $n := 2\ell+1$ if $\mathfrak{g}$ has type B_ℓ and $n := 2\ell$ if $\mathfrak{g}$ has type D_ℓ. Denote by $(n_1,\dots,n_k)$, with $n_1\geq\cdots\geq n_k$, the partition of n corresponding to the nilpotent element e. By [Mo06c, Théorème 1.1.8] or [Y06b], $\mathfrak{z}(\mathfrak{g}^e)$ is *not* generated by powers of e if and only if n_1 and n_2 are both odd integers and $n_3 < n_2$. On the other hand, since e is rigid, n_k is equal to 1, $n_i \leq n_{i+1} \leq n_i+1$ and all odd integers of the partition $(n_1,\dots,n_k)$ have a multiplicity different from 2 [Ke83, Sp82, ch. II] or [CMa93, Corollary 7.3.5]. Hence, the preceding criterion is not satisfied for e. Then, the second assertion results from Lemma 5.2, Corollary 4.16(i) and Theorem 4.13. □

Remark 5.4. Yakimova's proof of Elashvili's conjecture in the classical case is shorter and more elementary [Y06a]. The results of Section 4 will serve the exceptional case in a more relevant way.

5.2. The exceptional case. We let in this subsection $\mathfrak{g}$ be simple of exceptional type and we assume that e is a nonzero rigid nilpotent element of $\mathfrak{g}$. The dimension of the center of centralizers of nilpotent elements has been recently described in [LT08, Theorem 4]. On the other hand, we have explicit computations for the rigid nilpotent orbits in the exceptional types due to A.G. Elashvili. These computations are collected in [Sp82, Appendix of Chap. II] and a complete version was published later in [E85b]. From all this, we observe that the center of $\mathfrak{g}^e$ has dimension 1 in most cases. In more details, we have:

Proposition 5.5. *Let e be nonzero rigid nilpotent element of $\mathfrak{g}$.*
(i) *Suppose that $\mathfrak{g}$ has type* G_2, F_4 *or* E_6. *Then* $\dim\mathfrak{z}(\mathfrak{g}^e)=1$.
(ii) *Suppose that $\mathfrak{g}$ has type* E_7. *If $\mathfrak{g}^e$ has dimension* 41, *then* $\dim\mathfrak{z}(\mathfrak{g}^e)=2$; *otherwise* $\dim\mathfrak{z}(\mathfrak{g}^e)=1$.
(iii) *Suppose that $\mathfrak{g}$ has type* E_8. *If $\mathfrak{g}^e$ has dimension* 112, 84, 76, *or* 46, *then* $\dim\mathfrak{z}(\mathfrak{g}^e)=2$, *if $\mathfrak{g}^e$ has dimension* 72, *then* $\dim\mathfrak{z}(\mathfrak{g}^e)=3$; *otherwise* $\dim\mathfrak{z}(\mathfrak{g}^e)=1$.

By Corollary 4.16(ii), $\operatorname{ind}\mathfrak{g}^e = \ell$ whenever $\dim\mathfrak{z}(\mathfrak{g}^e) = 1$. So, as an immediate consequence of Proposition 5.5, we obtain:

COROLLARY 5.6. *Suppose that either* $\mathfrak{g}$ *has type* G_2, F_4, E_6, *or* $\mathfrak{g}$ *has type* E_7 *and* $\dim\mathfrak{g}^e \neq 41$, *or* $\mathfrak{g}$ *has type* E_8 *and* $\dim\mathfrak{g}^e \not\in \{112, 84, 76, 72, 46\}$. *Then* $\dim\mathfrak{z}(\mathfrak{g}^e) = 1$ *and the index of* $\mathfrak{g}^e$ *is equal to* ℓ.

According to Corollary 5.6, it remains 7 cases; there are indeed two rigid nilpotent orbits of codimension 46 in E_8. We handle now these remaining cases. We process here in a different way; we study technical conditions on $\mathfrak{g}^e$ under which $\operatorname{ind}\mathfrak{g}^e = \ell$. For the moment, we state general results about the index.

Let $\mathfrak{a}$ be an algebraic Lie algebra. Recall that the stabilizer of $\xi \in \mathfrak{a}^*$ for the coadjoint representation is denoted by $\mathfrak{a}^\xi$ and that ξ is regular if $\dim\mathfrak{a}^\xi = \operatorname{ind}\mathfrak{a}$. Choose a commutative subalgebra $\mathfrak{t}$ of $\mathfrak{a}$ consisted of semisimple elements of $\mathfrak{a}$ and denote by $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})$ the centralizer of $\mathfrak{t}$ in $\mathfrak{a}$. Then $\mathfrak{a} = \mathfrak{z}_\mathfrak{a}(\mathfrak{t}) \oplus [\mathfrak{t}, \mathfrak{a}]$. The dual $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ of $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})$ identifies to the orthogonal complement of $[\mathfrak{t}, \mathfrak{a}]$ in $\mathfrak{a}^*$. Thus, $\xi \in \mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ if and only if $\mathfrak{t}$ is contained in $\mathfrak{a}^\xi$.

LEMMA 5.7. *Suppose that there exists* ξ *in* $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ *such that* $\dim(\mathfrak{a}^\xi \cap [\mathfrak{t}, \mathfrak{a}]) \leq 2$. *Then*

$$\operatorname{ind}\mathfrak{a} \leq \operatorname{ind}\mathfrak{z}_\mathfrak{a}(\mathfrak{t}) + 1.$$

Proof. Let T be the closure in $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^* \times \mathrm{Gr}_3([\mathfrak{t}, \mathfrak{a}])$ of the subset of elements (η, E) such that η is a regular element of $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ and E is contained in $\mathfrak{a}^\eta$. The image T_1 of T by the projection from $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^* \times \mathrm{Gr}_3([\mathfrak{t}, \mathfrak{a}])$ to $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ is closed in $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$. By hypothesis, T_1 is not equal to $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ since for all η in T_1, $\dim(\mathfrak{a}^\eta \cap [\mathfrak{t}, \mathfrak{a}]) \geq 3$. Hence there exists a regular element ξ_0 in $\mathfrak{z}_\mathfrak{a}(\mathfrak{t})^*$ such that $\dim(\mathfrak{a}^{\xi_0} \cap [\mathfrak{t}, \mathfrak{a}]) \leq 2$. Since $\mathfrak{t}$ is contained in $\mathfrak{a}^{\xi_0}$,

$$\mathfrak{a}^{\xi_0} = \mathfrak{z}_\mathfrak{a}(\mathfrak{t})^{\xi_0} \oplus \mathfrak{a}^{\xi_0} \cap [\mathfrak{t}, \mathfrak{a}].$$

If $[\mathfrak{t}, \mathfrak{a}] \cap \mathfrak{a}^{\xi_0} = \{0\}$ then $\operatorname{ind}\mathfrak{a}$ is at most $\operatorname{ind}\mathfrak{z}_\mathfrak{a}(\mathfrak{t})$. Otherwise, $\mathfrak{a}^{\xi_0}$ is not a commutative subalgebra since $\mathfrak{t}$ is contained in $\mathfrak{a}^{\xi_0}$. Hence ξ_0 is not a regular element of $\mathfrak{a}^*$, so $\operatorname{ind}\mathfrak{a} < \dim\mathfrak{a}^{\xi_0}$. Since $\dim\mathfrak{a}^{\xi_0} \leq \operatorname{ind}\mathfrak{z}_\mathfrak{a}(\mathfrak{t}) + 2$, the lemma follows. □

From now on, we assume that $\mathfrak{a} = \mathfrak{g}^e$. As a rigid nilpotent element of $\mathfrak{g}$, e is a nondistinguished nilpotent element. So we can choose a nonzero commutative subalgebra $\mathfrak{t}$ of $\mathfrak{g}^e$ consisted of semisimple elements. Denote by $\mathfrak{l}$ the centralizer of $\mathfrak{t}$ in $\mathfrak{g}$. As a Levi subalgebra of $\mathfrak{g}$, $\mathfrak{l}$ is a reductive Lie algebra whose rank is ℓ. Moreover its dimension is strictly smaller than $\dim\mathfrak{g}$. In the preceding notations, we have $\mathfrak{z}_{\mathfrak{g}^e}(\mathfrak{t}) = \mathfrak{z}_\mathfrak{g}(\mathfrak{t})^e = \mathfrak{l}^e$. Let $\mathfrak{t}_1$ be a commutative subalgebra of $\mathfrak{l}^e$ containing $\mathfrak{t}$ and consisting of semisimple elements of $\mathfrak{l}$. Then $[\mathfrak{t},\mathfrak{g}^e]$ is stable under the adjoint action of $\mathfrak{t}_1$. For λ in $\mathfrak{t}_1^*$, denote by $\mathfrak{g}^e_\lambda$ the λ-weight space of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^e$.

Lemma 5.8. *Let $\lambda \in \mathfrak{t}_1^*$ be a nonzero weight of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^e$. Then $-\lambda$ is also a weight for this action and λ and $-\lambda$ have the same multiplicity. Moreover, $\mathfrak{g}^e_\lambda$ is contained in $[\mathfrak{t},\mathfrak{g}^e]$ if and only if the restriction of λ to $\mathfrak{t}$ is not identically zero.*

Proof. By definition, $\mathfrak{g}^e_\lambda \cap \mathfrak{l}^e = \{0\}$ if and only if the restriction of λ to $\mathfrak{t}$ is not identically zero. So $\mathfrak{g}^e_\lambda$ is contained in $[\mathfrak{t},\mathfrak{g}^e]$ if and only if the restriction of λ to $\mathfrak{t}$ is not equal to 0 since

$$\mathfrak{g}^e_\lambda = (\mathfrak{g}^e_\lambda \cap \mathfrak{l}^e) \oplus (\mathfrak{g}^e_\lambda \cap [\mathfrak{t},\mathfrak{g}^e]).$$

The subalgebra $\mathfrak{t}_1$ is contained in a reductive factor of $\mathfrak{g}^e$. So we can choose h and f such that $\mathfrak{t}_1$ is contained in $\mathfrak{g}^e \cap \mathfrak{g}^f$. As a consequence, any weight of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^f$ is a weight of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^e$ with the same multiplicity. Furthermore, the $\mathfrak{t}_1$-module $\mathfrak{g}^f$ for the ajoint action is isomorphic to the $\mathfrak{t}_1$-module $(\mathfrak{g}^e)^*$ for the coadjoint action. So $-\lambda$ is a weight of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^f$ with the same multiplicity as λ. Hence $-\lambda$ is a weight of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^e$ with the same multiplicity as λ, whence the lemma. □

Choose pairwise different elements $\lambda_1,\dots,\lambda_r$ of $\mathfrak{t}_1^*$ so that the weights of the adjoint action of $\mathfrak{t}_1$ in $\mathfrak{g}^e$ which are not identically zero on $\mathfrak{t}$ are precisely the elements $\pm\lambda_i$. For $i = 1,\dots,r$, let $v_{i,1},\dots,v_{i,m_i}$ and $w_{i,1},\dots,w_{i,m_i}$ be basis of $\mathfrak{g}^e_{\lambda_i}$ and $\mathfrak{g}^e_{-\lambda_i}$ respectively. Then we set:

$$q_i := \det\left([v_{i,k}, w_{i,l}]\right)_{1\leq k,l\leq m_i} \in \mathrm{S}(\mathfrak{l}^e).$$

Proposition 5.9. *Suppose that* $\operatorname{ind}\mathfrak{l}^e = \ell$ *and suppose that one of the following two conditions is satisfied:*

1. *for $i = 1,\dots,r$, $q_i \neq 0$,*
2. *there exists j in $\{1,\dots,r\}$ such that $q_i \neq 0$ for all $i \neq j$ and such that the basis $v_{j,1},\dots,v_{j,m_j}$ and $w_{j,1},\dots,w_{j,m_j}$ can be chosen so that*

$$\det\left([v_{j,k}, w_{j,l}]\right)_{1\leq k,l\leq m_j-1} \neq 0.$$

Then, $\operatorname{ind}\mathfrak{g}^e = \ell$.

Proof. First, observe that $\operatorname{ind}\mathfrak{g}^e - \operatorname{ind}\mathfrak{g}$ is an even integer. Indeed, we have:

$$\operatorname{ind}\mathfrak{g}^e - \operatorname{ind}\mathfrak{g} = (\operatorname{ind}\mathfrak{g}^e - \dim\mathfrak{g}^e) + (\dim\mathfrak{g}^e - \dim\mathfrak{g}) + (\dim\mathfrak{g} - \operatorname{ind}\mathfrak{g}).$$

But the integers $\operatorname{ind}\mathfrak{g}^e - \dim\mathfrak{g}^e$, $\dim\mathfrak{g}^e - \dim\mathfrak{g}$ and $\dim\mathfrak{g} - \operatorname{ind}\mathfrak{g}$ are all even integers. Thereby, if $\operatorname{ind}\mathfrak{g}^e \leq \operatorname{ind}\mathfrak{g} + 1$, then $\operatorname{ind}\mathfrak{g}^e \leq \operatorname{ind}\mathfrak{g}$. In

turn, by Vinberg's inequality (cf. Introduction), we have $\operatorname{ind}\mathfrak{g}^e \geq \operatorname{ind}\mathfrak{g}$. Hence, it suffices to prove $\operatorname{ind}\mathfrak{g}^e \leq \operatorname{ind}\mathfrak{l}^e + 1$ since our hypothesis says that $\operatorname{ind}\mathfrak{l}^e = \ell = \operatorname{ind}\mathfrak{g}$. Now, by Lemma 5.7, if there exists ξ in $(\mathfrak{l}^e)^*$ such that $(\mathfrak{g}^e)^\xi \cap [\mathfrak{t}, \mathfrak{g}^e]$ has dimension at most 2, then we are done.
Denote by $\mathfrak{l}_1$ the centralizer of $\mathfrak{t}_1$ in $\mathfrak{g}$. Then $\mathfrak{l}_1$ is contained in $\mathfrak{l}$ and $\mathfrak{l}^e = \mathfrak{l}_1^e \oplus [\mathfrak{t}_1, \mathfrak{l}^e]$ and $(\mathfrak{l}_1^e)^*$ identifies to the orthogonal of $[\mathfrak{t}_1, \mathfrak{l}^e]$ in the dual of $\mathfrak{l}^e$. Moreover, for $i = 1, \ldots, r$, q_i belongs to $\mathrm{S}(\mathfrak{l}_1^e)$. For ξ in $(\mathfrak{l}_1^e)^*$, denote by B_ξ the bilinear form

$$\begin{array}{ccc} [\mathfrak{t}, \mathfrak{g}^e] \times [\mathfrak{t}, \mathfrak{g}^e] & \longrightarrow & \Bbbk \\ (v, w) & \longmapsto & \xi([v, w]) \end{array}$$

and denote by $\ker B_\xi$ its kernel. For $i = 1, \ldots, r$, $-q_i(\xi)^2$ is the determinant of the restriction of B_ξ to the subspace

$$(\mathfrak{g}^e_{\lambda_i} \oplus \mathfrak{g}^e_{-\lambda_i}) \times (\mathfrak{g}^e_{\lambda_i} \oplus \mathfrak{g}^e_{-\lambda_i})$$

in the basis $v_{i,1}, \ldots, v_{i,m_i}, w_{i,1}, \ldots, w_{i,m_i}$.
If (1) holds, we can find ξ in $(\mathfrak{l}_1^e)^*$ such that $\ker B_\xi$ is zero. If (2) holds, we can find ξ in $(\mathfrak{l}_1^e)^*$ such that $\ker B_\xi$ has dimension 2 since B_ξ is invariant under the adjoint action of $\mathfrak{t}_1$. But $\ker B_\xi$ is equal to $(\mathfrak{g}^e)^\xi \cap [\mathfrak{t}, \mathfrak{g}^e]$. Hence such a ξ satisfies the required inequality and the proposition follows. □

The proof of the following proposition is given in Appendix A since it relies on explicit computations:

PROPOSITION 5.10. (i) *Suppose that either* $\mathfrak{g}$ *has type* E_7 *and* $\dim\mathfrak{g}^e = 41$ *or,* $\mathfrak{g}$ *has type* E_8 *and* $\dim\mathfrak{g}^e \in \{112, 72\}$*. Then, for suitable choices of* $\mathfrak{t}$ *and* $\mathfrak{t}_1$*, Condition* (1) *of Proposition* 5.9 *is satisfied.*
(ii) *Suppose that* $\mathfrak{g}$ *has type* E_8 *and that* $\mathfrak{g}^e$ *has dimension* 84, 76*, or* 46*. Then, for suitable choices of* $\mathfrak{t}$ *and* $\mathfrak{t}_1$*, Condition* (2) *of Proposition* 5.5 *is satisfied.*

5.3. PROOF OF THEOREM 1.3. We are now in position to complete the proof of Theorem 1.3:

Proof of Theorem 1.3. We argue by induction on the dimension of $\mathfrak{g}$. If $\mathfrak{g}$ has dimension 3, the statement is known. Assume now that $\operatorname{ind}\mathfrak{l}^{e'} = \operatorname{rk}\mathfrak{l}$ for any reductive Lie algebras $\mathfrak{l}$ of dimension at most $\dim\mathfrak{g} - 1$ and any $e' \in \mathcal{N}(\mathfrak{l})$. Let $e \in \mathcal{N}(\mathfrak{g})$ be a nilpotent element of $\mathfrak{g}$. By Theorem 3.3 and Theorem 5.3, we can assume that e is rigid and that $\mathfrak{g}$ is simple of exceptional type. Furthermore by Corollary 5.6, we can assume that $\dim\mathfrak{z}(\mathfrak{g}^e) > 1$. Then we consider the different cases given by Proposition 5.10.
If, either $\mathfrak{g}$ has type E_7 and $\dim\mathfrak{g}^e = 41$, or $\mathfrak{g}$ has type E_8 and $\dim\mathfrak{g}^e$ equals 112, 72, or 46, then Condition (1) of Proposition 5.9 applies for

suitable choices of $\mathfrak{t}$ and $\mathfrak{t}_1$ by Proposition 5.10. Moreover, if $\mathfrak{l} = \mathfrak{z}_{\mathfrak{g}}(\mathfrak{t})$, then $\mathfrak{l}$ is a reductive Lie algebra of rank ℓ and strictly contained in $\mathfrak{g}$. So, from our induction hypothesis, we deduce that $\operatorname{ind}\mathfrak{g}^e = \ell$ by Proposition 5.9.
If $\mathfrak{g}$ has type E_8 and $\dim\mathfrak{g}^e$ equals 84, 76, or 46, then Condition (2) of Proposition 5.9 applies for suitable choices of $\mathfrak{t}$ and $\mathfrak{t}_1$ by Proposition 5.10. Arguing as above, we deduce that $\operatorname{ind}\mathfrak{g}^e = \ell$. □

Appendix A. Proof of Proposition 5.10: explicit computations.

This appendix aims to prove Proposition 5.10. We prove Proposition 5.10 for each case by using explicit computations made with the help of `GAP`; our programmes are presented below (two cases are detailed; the other ones are similar). Explain the general approach. In our programmes, $x[1], \ldots$ are root vectors generating the nilradical of the Borel subalgebra $\mathfrak{b}$ of $\mathfrak{g}$ and the representative e (denoted by `e` in our programmes) of the rigid orbit is chosen so that e and h belong to $\mathfrak{b}$ and $\mathfrak{h}$ respectively. The element e is given by the tables of [GQT80]. In fact, in [GQT80], they use the programme Lie which induces minor changes in the numbering. Then, we exhibit suitable tori $\mathfrak{t}$ and $\mathfrak{t}_1$ of $\mathfrak{g}$ contained in $\mathfrak{g}^e$ which satisfies conditions (1) or (2) of Proposition 5.9. In each case, our torus $\mathfrak{t}$ is one dimensional; we define it by a generator, called `t` in our programmes. Its centralizer in $\mathfrak{g}^e$ is denoted by `le`. The torus $\mathfrak{t}_1$ has dimension at most 4. It is defined by a basis denoted by `Bt1`. The weights of $\mathfrak{t}_1$ for the adjoint action of $\mathfrak{t}_1$ on $\mathfrak{g}^e$ are given by their values on the basis `Bt1` of $\mathfrak{t}_1$. We list in a matrix `W` almost all weights which have a positive value at `Bt1`. The other weights have multiplicity 1. In our programmes, by the term `S` we check that no weight is forgotten; this term has to be zero. Then, the matrices corresponding to the weights given by `W` are given by a function `A`. Their determinants correspond to the q_i's in the notations of Proposition 5.9. If there is only one other weight, the corresponding matrix is denoted by `a`. At last, we verify that these matrices have the desired property depending on the situations (i) or (ii) of Proposition 5.10.
As examples, we detail below two cases:
(1) the case of E_7 with $\dim\mathfrak{g}^e = 41$ where we intend to check that Condition (1) of Proposition 5.9 is satisfied;
(2) the case of E_8 with $\dim\mathfrak{g}^e = 84$ where we intend to check that Condition (2) of Proposition 5.9 is satisfied.

(1) E_7, $\dim \mathfrak{g}^e = 41$: In this case, with our choices, $\dim \mathfrak{t} = 1$, $\dim \mathfrak{l}^e = 23$ and $\dim \mathfrak{t}_1 = 3$. The order of matrices to be considered is at most 2.

```
L := SimpleLieAlgebra("E",7,Rationals);;
R := RootSystem(L);;
x := PositiveRootVectors(R);; y := NegativeRootVectors(R);;
e := x[14]+x[26]+x[28]+x[49];;
c := LieCentralizer(L,Subspace(L,[e]));
Bc := BasisVectors(Basis(c));;
> <Lie algebra of dimension 41 over Rationals>
z := LieCentre(c);; Bz := BasisVectors(Basis(z));;
t := Bc[Dimension(c)];;
le := LieCentralizer(L,Subspace(L,[t,e]));
> <Lie algebra of dimension 23 over Rationals>
n := function(k)
     if k=2 then return 1;;
     elif k=-2 then return 1;;
     elif k=1 then return 8;;
     elif k=-1 then return 8;; fi;; end;;
#The function n assigns to each weight of t
#the dimension of the corresponding
#weight subspace.
M := function(k)  local m;;
   m := function(j,k)
      if j=1 then
          return Position(List([1..Dimension(c)],
              i->t*Bc[i]-k*Bc[i]),0*x[1]);;
          else
             return m(j-1,k)
                 +Position(List([m(j-1,k)+1..Dimension(c)],
          i->t*Bc[i]-k*Bc[i]),0*x[1]);;
          fi;;
     end;;
     return List([1..n(k)],i->m(i,k));;
end;;
Bt1 := [Bc[41],Bc[40],Bc[39]];;
N := function(k,p) local n;;
     n := function(j,k,p)
          if j=1 then
              return Position(List([1..8],
          i->Bt1[2]*Bc[M(k)[i]]-p*Bc[M(k)[i]]),0*x[1]);;
          else
```

```
              return n(j-1,k,p)
                   +Position(List([n(j-1,k,p)+1..8],
          i->Bt1[2]*Bc[M(k)[i]]-p*Bc[M(k)[i]]),0*x[1]);;
          fi;;
     end;;
     return List([1..4],i->M(k)[n(i,k,p)]);;
end;;
r := function(t)
     if t=1 then return 1;
     elif t=-1 then return 1;;
     elif t=0 then return 2;;
     fi;;
end;;
Q := function(k,s,t) local q;;
  q := function(j,k,s,t)
     if j=1 then
          return Position(List([1..4],
     i->Bt1[3]*Bc[N(k,s)[i]]-t*Bc[N(k,s)[i]]),0*x[1]);;
     else
          return q(j-1,k,s,t)
                  +Position(List([q(j-1,k,s,t)+1..4],
     i->Bt1[3]*Bc[N(k,s)[i]]-t*Bc[N(k,s)[i]]),0*x[1]);;
          fi;;
     end;;
     return List([1..r(t)],i->N(k,s)[q(i,k,s,t)]);;
end;;
W := [[1,1,1],[1,-1,1],[1,1,-1],[1,-1,-1],
                               [1,1,0],[1,-1,0]];;
S := 2*(1+Sum(List([1..Length(W)],
                i->Length(Q(W[i][1],W[i][2],W[i][3])))))
                    +Dimension(le)-Dimension(c);
> 0
A := function(i) return
          List([1..r(W[i][3])],t->List([1..r(W[i][3])],
     s->Bc[Q(W[i][1],W[i][2],W[i][3])[s]]*
                Bc[Q(-W[i][1],-W[i][2],-W[i][3])[t]]));;
end;;
A(1);A(2);A(3);A(4);A(5);A(6);
> [ [ (-1)*v.63 ] ]
> [ [ v.63 ] ]
> [ [ v.63 ] ]
```

```
> [ [ (-1)*v.63 ] ]
> [ [ (-1)*v.57+(-1)*v.60, (-1)*v.63 ],
                           [ (-1)*v.63, 0*v.1 ] ]
> [ [ (-1)*v.57+(-1)*v.60, (-1)*v.63 ],
                              [ (-1)*v.63, 0*v.1 ] ]
a := Bc[M(2)[1]]*Bc[M(-2)[1]];
> v.133
```

In conclusion, Condition (1) of Proposition 5.9 is satisfied for $\mathfrak{t} := \Bbbk$t and $\mathfrak{t}_1$:=span(Bt1).

(2) E_8, $\dim \mathfrak{g}^e = 84$: In this case, with our choices, $\dim \mathfrak{t} = 1$, $\dim \mathfrak{l}^e = 48$ and $\dim \mathfrak{t}_1 = 3$. The matrix `A(7)` has order 5 and it is singular of rank 4. The order of the other matrices is at most 2.

```
L := SimpleLieAlgebra("E",8,Rationals);;
R := RootSystem(L);;
x := PositiveRootVectors(R);; y := NegativeRootVectors(R);;
e := x[54]+x[61]+x[77]+x[97];;
c := LieCentralizer(L,Subspace(L,[e]));
Bc := BasisVectors(Basis(c));;
> <Lie algebra of dimension 84 over Rationals>
z := LieCentre(c);; Bz := BasisVectors(Basis(z));;
t := Bc[Dimension(c)];;
le := LieCentralizer(L,Subspace(L,[t,e]));
> <Lie algebra of dimension 48 over Rationals>
n := function(k)
     if k=2 then return 1;;
     elif k=-2 then return 1;;
     elif k=1 then return 17;;
     elif k=-1 then return 17;;
     fi;;
end;;
M := function(k)  local m;;
   m := function(j,k)
      if j=1 then
          return Position(List([1..Dimension(c)],
        i->Bc[84]*Bc[i]-k*Bc[i]),0*x[1]);;
      else
          return m(j-1,k)
            +Position(List([m(j-1,k)+1..Dimension(c)],
          i->Bc[84]*Bc[i]-k*Bc[i]), 0*x[1]);;
          fi;;
```

```
     end;;
     return List([1..n(k)],i->m(i,k));;
end;;
r := function(k,t)
     if k=1 and t=1  then return 4;;
     elif k=-1 and t=-1  then return 4;;
     elif k=1 and t=-1  then return 4;;
     elif k=-1 and t=1  then return 4;;
     elif k=1 and t=0  then return 9;;
     elif k=-1 and t=0  then return 9;;
     fi;;
end;;
Bt1 := [Bc[84],Bc[83],Bc[82]];;
N := function(k,t) local p;;
   p := function(j,k,t)
      if j=1 then
         return Position(List([1..n(k)],
       i->Bt1[2]*Bc[M(k)[i]]-t*Bc[M(k)[i]]),0*x[1]);;
      else
         return p(j-1,k,t)
              +Position(List([p(j-1,k,t)+1..n(k)],
       i->Bt1[2]*Bc[M(k)[i]]-t*Bc[M(k)[i]]),0*x[1]);;
          fi;;
     end;;
     return List([1..r(k,t)],i->M(k)[p(i,k,t)]);;
end;;
m := function(k,s,t)
     if k=1 and s=1 and t=-1 then return 2;;
     elif k=-1 and s=-1 and t=1 then  return 2;;
     elif k=1 and s=1 and t=0 then return 2;;
     elif k=-1 and s=-1 and t=0 then return 2;;
     elif k=1 and s=-1 and t=1 then  return 2;;
     elif k=-1 and s=1 and t=-1 then return 2;;
     elif k=1 and s=-1 and t=0 then return 2;;
     elif k=-1 and s=1 and t=0 then  return 2;;
     elif k=1 and s=0 and t=1 then return 2;;
     elif k=-1 and s=0 and t=-1 then return 2;;
     elif k=1 and s=0 and t=-1 then return 2;;
     elif k=-1 and s=0 and t=1 then return 2;;
     elif k=1 and s=0 and t=0 then return 5;;
     elif k=-1 and s=0 and t=0 then return 5;;
```

```
     fi;;
end;;
Q := function(k,s,t) local q;;
  q := function(j,k,s,t)
    if j=1 then
        return Position(List([1..r(k,s)],
     i->Bt1[3]*Bc[N(k,s)[i]]-t*Bc[N(k,s)[i]]),0*x[1]);;
    else
        return q(j-1,k,s,t)
              +Position(List([q(j-1,k,s,t)+1..r(k,s)],
     i->Bt1[3]*Bc[N(k,s)[i]]-t*Bc[N(k,s)[i]]),0*x[1]);;
         fi;;
     end;;
     return List([1..m(k,s,t)],i->N(k,s)[q(i,k,s,t)]);;
end;;
W := [[1,1,-1],[1,1,0],[1,-1,1],[1,-1,0],
                        [1,0,1],[1,0,-1],[1,0,0]];;
S := 2 + 2*Sum(List([1..Length(W)],
               i->Length(Q(W[i][1],W[i][2],W[i][3]))))
                  + Dimension(le)-Dimension(c);;
A := function(i) return
     List([1..m(W[i][1],W[i][2],W[i][3])],
        t->List([1..m(W[i][1],W[i][2],W[i][3])],
        s->Bc[Q(W[i][1],W[i][2],W[i][3])[s]]*
               Bc[Q(-W[i][1],-W[i][2],-W[i][3])[t]]));;
end;;
# A(1), A(2), A(3), A(5), A(6) are nonsingular.
# A(7) is singular of order 5 of rank 4; its minor
List([1..4],s->List([1..4],
t->Bc[Q(W[7][1],W[7][2],W[7][3])[s]]*
              Bc[Q(-W[7][1],-W[7][2],-W[7][3])[t]]));;
# is different from 0.
a := Bc[M(2)[1]]*Bc[M(-2)[1]];;
```

In conclusion, Condition (2) of Proposition 5.9 is satisfied for $\mathfrak{t} := \Bbbk\mathtt{t}$ and $\mathfrak{t}_1$:=span(Bt1).

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The Cohomology Rings of Moduli Stacks of Principal Bundles over Curves

Dedicated with gratitude
to the memory of Eckart Viehweg

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Abstract. We prove that the cohomology of the moduli stack of G-bundles on a smooth projective curve is freely generated by the Atiyah–Bott classes in arbitrary characteristic. The main technical tool needed is the construction of coarse moduli spaces for bundles with parabolic structure in arbitrary characteristic. Using these spaces we show that the cohomology of the moduli stack is pure and satisfies base-change for curves defined over a discrete valuation ring. Thereby we get an algebraic proof of the theorem of Atiyah and Bott and conversely this can be used to give a geometric proof of the fact that the Tamagawa number of a Chevalley group is the number of connected components of the moduli stack of principal bundles.

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Contents

1 Introduction

Atiyah and Bott [1] proved that for any semisimple group G the cohomology ring of the moduli stack Bun_G of principal G-bundles on a Riemann surface C is freely generated by the Künneth components of the characteristic classes of the universal bundle on $\mathrm{Bun}_G \times C$. (Of course, in their article, this was expressed in terms of equivariant cohomology instead of the cohomology of a stack. The formulation in terms of stacks can also be found in Teleman's article [42].) The argument of Harder and Narasimhan [19] suggests that the result should also hold for curves over finite fields.

The original aim of this article was to give an algebraic proof of the result of Atiyah and Bott in positive characteristics. In the case of $G = \mathrm{GL}_n$ this was suggested by G. Harder, given as a Diploma thesis to the first author [21] (see [10] for a different approach). For general G we have to use the recent constructions of coarse moduli spaces in arbitrary characteristics [15]. The results of Behrend ([4], [5]) prove the Lefschetz trace formula for the moduli stack Bun_G over finite fields. However, purity of the cohomology groups is not so clear. One also has to check that the universal classes generate a sufficiently large subring. To prove purity, we embed the cohomology of the stack into the cohomology of a projective variety. This enables us to argue in two ways: either we use the known calculations of the Tamagawa number to prove the theorem with algebraic methods over finite fields (Theorem 3.3.5), or we use the projective variety to apply base change (Corollary 3.3.4) and deduce the

general result from the known one in characteristic 0. This in turn gives a calculation of the Tamagawa number (Corollary 3.1.3) and thus provides a geometric proof of Harder's conjecture that the Tamagawa number should be the number of connected components of the moduli stack of principal G-bundles in this situation (see also the introduction to [8]). In order to make this argument precise the formalism of the six operations for sheaves on Artin stacks recently constructed by Laszlo and Olsson [29] is applied.
As pointed out by Neumann and Stuhler in [33], the computation of the cohomology ring over finite fields also gives an explicit description of the action of the Frobenius endomorphism of the moduli stack on the cohomology of the stack, even if the geometry of this action is quite mysterious.
As explained above, the main new ingredient in our approach is the purity of the cohomology and the proof of a base change theorem for the cohomology of Bun_G. The idea to prove these results is to embed the cohomology of Bun_G into the cohomology of the stack of principal G-bundles together with flags at a finite set of points of the curve ("flagged principal bundles"). On this stack one can find a line bundle, such that the open subset of stable bundles has a complement of high codimension. Furthermore, there exists a projective coarse moduli space for stable flagged principal bundles. The existence of coarse moduli spaces for flagged principal bundles in arbitrary characteristic is demonstrated in the second part of this article. So here we use Geometric Invariant Theory in order to obtain a result for the moduli stack, whereas one usually argues in the other direction.
Our main theorem is:

Theorem. *Assume that C is a curve over a field k. Then the cohomology of the connected components Bun_G^ϑ of Bun_G is freely generated by the canonical classes, i.e.,*

$$H^\star\big(\mathrm{Bun}^\vartheta_{G,\overline{k}},\overline{\mathbb{Q}}_\ell\big)=\overline{\mathbb{Q}}_\ell[a_1,\ldots,a_r]\otimes\bigwedge^{\star}[b_i^j]_{i=1,\ldots r,j=1,\ldots,2g}\otimes\overline{\mathbb{Q}}_\ell[f_1,\ldots,f_r].$$

(The canonical classes are obtained from the Künneth components of the universal principal bundle on $\mathrm{Bun}_G\times C$, see Section 3.1.)
As remarked above, the main technical ingredient is the construction of proper coarse moduli spaces for flagged principal bundles in positive characteristic. It is contained in the second part of this paper and might be of independent interest. Let us therefore give a statement of this result as well.
Since there are different definitions of parabolic bundles in the literature, we have used the term flagged principal bundles instead. The precise definition is as follows. Let $\underline{x}=(x_i)_{i=1,\ldots,b}$ be a finite set of distinct k-rational points of C, and let $\underline{P}=(P_i)_{i=1,\ldots,b}$ be a tuple of parabolic subgroups of G. A *principal G-bundle with a flagging of type* $(\underline{x},\underline{P})$ is a tuple $(\mathscr{P},\underline{s})$ that consists of a principal G-bundle $\mathscr{P}$ on C and a tuple $\underline{s}=(s_1,\ldots,s_b)$ of sections $s_i\colon\{x_i\}\to(\mathscr{P}\times_C\{x_i\})/P_i$, i.e., s_i is a reduction of the structure group of $\mathscr{P}\times_C\{x_i\}$ to P_i, $i=1,\ldots,b$.

In Section 4 we introduce a semistability concept for such bundles. It depends on a parameter $\underline{a}$ which, as in the case of parabolic vector bundles, has to satisfy a certain admissibility condition. Using this notion we show:

Theorem. *For any type* $(\underline{x},\underline{P})$ *of flaggings and any admissible stability parameter* $\underline{a}$*, there exists a projective coarse moduli space* $\mathscr{M}(\underline{x},\underline{P})^{\underline{a}\text{-ss}}$ *of* $\underline{a}$*-semistable flagged principal* G*-bundles.*

Finally one should note that it is well known that one can use the computation of the cohomology of the moduli stack and the splitting of the Gysin sequence for the Harder–Narasimhan stratification of Bun_G (as in [1], this holds in arbitrary characteristic) to calculate the cohomology of the moduli stack of semistable bundles. If the connected component $\mathrm{Bun}_G^{\vartheta}$ is such that there are no properly semistable bundles, this gives a computation of the cohomology of the coarse moduli space (as in the proof of Corollary 3.3.2).

2 Preliminaries

In this section we collect some well known results on the moduli stacks Bun_G and their cohomology.

2.1 Basic Properties of the Moduli Stack of Principal Bundles

Let C be a smooth, projective curve of genus g over the (locally noetherian) scheme S. It would be reasonable to assume that C is a curve over a field, but since we want to be able to transport our results from characteristic p to characteristic 0, we will finally need some base ring.
Let G/S be a reductive group of rank r. Denote by Bun_G the moduli stack of principal G-bundles over C, i.e., for a scheme $X \to S$, the X-valued points of Bun_G are defined as

$$\mathrm{Bun}_G(X) := \text{Category of principal } G\text{-bundles over } C \times X.$$

Recall the following basic fact which is proved in [4], Proposition 4.4.6 and Corollary 4.5.2.

Proposition 2.1.1. *The stack* Bun_G *is an algebraic stack, locally of finite type and smooth of relative dimension* $(g-1)\dim G$ *over* S*.*

Furthermore the connected components of Bun_G are known ([14], Proposition 5, [24]). (In the first reference, the result is stated only for simply connected groups, but the proof gives the result in the general case.)

Proposition 2.1.2. *If* $S = \mathrm{Spec}(\overline{k})$*, or if* G *is a split reductive group, then the connected components of* Bun_G *are in natural bijection to* $\pi_1(G)$*.*

Remark 2.1.3. The stack Bun_G is smooth (2.1.1). Therefore, its connected components are also irreducible.

2.2 Behrend's Trace Formula

Let us now assume that $S = \mathrm{Spec}(k)$ is the spectrum of a field. In the following, we will write $\mathrm{Bun}^{\vartheta}_{G,\overline{k}}$ with $\vartheta \in \pi_1(G_{\overline{k}})$ for the corresponding connected component of $\mathrm{Bun}_{G,\overline{k}}$.

Since the stack $\mathrm{Bun}_G^{\vartheta}$ is only locally of finite type, we define its ℓ-adic cohomology as the limit of the cohomologies of all open substacks of finite type:

$$H^\star(\mathrm{Bun}_G^{\vartheta}, \overline{\mathbb{Q}}_\ell) := \lim_{\substack{U\subset \mathrm{Bun}_G \\ \text{open, fin. type}}} H^\star(U, \overline{\mathbb{Q}}_\ell).$$

Remark 2.2.1. The basic reference for stacks and their cohomology is [30]. The general formalism of cohomology has been developed in the articles by Laszlo and Olsson [29]. Behrend in [7] also constructed all the functors that we will use. In particular, we will compute cohomology groups with respect to the lisse-étale topology. To simplify the statement of our main theorem we will use $\overline{\mathbb{Q}}_\ell$ coefficients, because we want to chose generators of the cohomology ring that are eigenvectors for the Frobenius action.

By semi-purity, which is recalled below, the cohomology of Bun_G in degrees $< 2i$ is equal to the cohomology of $U \subset \mathrm{Bun}_G$, if the codimension of the complement of U is at least i:

Lemma 2.2.2 (Semi-purity). *Let X be a smooth stack of finite type and $U \overset{j}{\hookrightarrow} X$ an open substack with complement $Z := X \setminus U \overset{i}{\hookrightarrow} X$. Then,*

$$H^\star(X, \overline{\mathbb{Q}}_\ell) \cong H^\star(U, \overline{\mathbb{Q}}_\ell) \quad \textit{for } \star < 2\,\mathrm{codim}(Z).$$

Proof. As usual, this can be deduced from the corresponding statement for schemes. For schemes instead of stacks, this follows from the long exact sequence for cohomology with compact support,

$$\cdots \longrightarrow H_c^\star(U, \overline{\mathbb{Q}}_\ell) \longrightarrow H_c^\star(X, \overline{\mathbb{Q}}_\ell) \longrightarrow H_c^\star(Z, \overline{\mathbb{Q}}_\ell) \longrightarrow \cdots,$$

the vanishing of $H_c^\star(Z, \overline{\mathbb{Q}}_\ell)$ for $\star > 2\dim Z$, and Poincaré duality,

$$H_c^{2\dim U - \star}(U, \overline{\mathbb{Q}}_\ell) \cong H^\star\big(U, \overline{\mathbb{Q}}_\ell(\dim U)\big)^\vee.$$

Now, if $X_0 \twoheadrightarrow X$ is a smooth atlas of the stack X, and $X_n := X_0 \times_X X_0 \times_X \cdots \times_X X_0$, then there is a spectral sequence:

$$H^p(X_q, \overline{\mathbb{Q}}_\ell) \Rightarrow H^{p+q}(X, \overline{\mathbb{Q}}_\ell).$$

Since the codimension is preserved under smooth pull-backs, for any $U \subset X$, we get the atlas $U_0 := U \times_X X_0 \to U$, and the induced embeddings $U_q \to X_q$ have complements of codimension $\mathrm{codim}(U)$. Therefore we can apply the lemma in the case of schemes to the morphism of spectral sequences

$$H^p(U_q, \overline{\mathbb{Q}}_\ell) \to H^p(X_q, \overline{\mathbb{Q}}_\ell)$$

to prove our claim. □

Remark 2.2.3. The same argument applies to the higher direct image sheaves in the relative situation $X \to S$, if X is smooth over S and $U \subset X$ is of codimension i in every fiber.

Behrend proved ([4], [5]) that, if C is a curve defined over a finite field k, the Lefschetz trace formula holds for the stack Bun_G.

Theorem 2.2.4 (Behrend). *Let C be a smooth, projective curve over the finite field $k = \mathbb{F}_q$ and G a semisimple group over k. Let* Frob *denote the arithmetic Frobenius acting on $H^\star(\mathrm{Bun}_{G,\overline{k}}, \overline{\mathbb{Q}}_\ell)$. Then, we have*

$$q^{\dim(\mathrm{Bun}_G)} \sum_{i \geq 0} (-1)^i \operatorname{tr}\big(\mathrm{Frob}, H^i(\mathrm{Bun}_{G,\overline{k}}, \overline{\mathbb{Q}}_\ell)\big) = \sum_{x \in \mathrm{Bun}_G(\mathbb{F}_q)} \frac{1}{\# \operatorname{Aut}(x)(\mathbb{F}_q)}.$$

As in [19], a result of Siegel allows us to calculate the right hand side of the formula. To state it, we first recall a theorem of Steinberg.

Proposition 2.2.5 (Steinberg). *Let G be a semisimple group over $k = \mathbb{F}_q$. There are integers $d_1, \dots, d_r$ and roots of unity $\epsilon_1, \dots, \epsilon_r$ such that:*

- $\#G(\mathbb{F}_q) = q^{\dim G} \prod_{i=1}^r (1 - \epsilon_i q^{-d_i})$
- *Let BG be the classifying stack of principal G-bundles. Then, $H^\star(BG_{\overline{k}}, \overline{\mathbb{Q}}_\ell) = \overline{\mathbb{Q}}_\ell[c_1, \dots, c_r]$ with $c_i \in H^{2d_i}(BG, \overline{\mathbb{Q}}_\ell)$ and* $\mathrm{Frob}(c_i) = \epsilon_i q^{-d_i}$.

The second part is of course not stated in this form in Steinberg's book [40], but one only has to recall the argument from topology. First the theorem holds for tori, since $H^\star(\mathbb{G}_m, \overline{\mathbb{Q}}_\ell) = \overline{\mathbb{Q}}_\ell[x]$. For a maximal torus T contained in the Borel subgroup $B \subset G$, the map $BT \to BB$ induces an isomorphism in cohomology: since the fibers are isomorphic to BU where $U \cong \mathbb{A}^n$ is the unipotent radical of B, they have no higher cohomology. The fibers of the map $BB \to BG$ are isomorphic to the flag manifold G/B. Thus the map $\mathrm{ind}_T^G \colon BT \to BG$ induces an injection $\mathrm{ind}_T^{G,\star} \colon H^\star(BG, \overline{\mathbb{Q}}_\ell) \hookrightarrow H^\star(BT, \overline{\mathbb{Q}}_\ell)$ which lies in the part invariant under the Weyl group. For dimensional reasons—since we already stated the trace formula, this follows most easily from $1/(\#G(\mathbb{F}_q)) = q^{-\dim G} \sum \operatorname{tr}(\mathrm{Frob}, H^i(BG_{\overline{k}}, \overline{\mathbb{Q}}_\ell))$ and the fact that the d_i are the degrees of the homogeneous generators in $H^\star(BT_{\overline{k}}, \overline{\mathbb{Q}}_\ell)^W$—it must then be isomorphic to the invariant ring.

With the notations from Steinberg's theorem we can state a theorem of Siegel. A nice reference for the theorem is [26], Section 3. In this article, you can also find a short reminder on the Tamagawa number $\tau(G)$.

Theorem 2.2.6 (Siegel's formula). *Let $G_{/\mathbb{F}_q}$ be a semisimple group, and denote* *by α_j the eigenvalues of the geometric Frobenius on $H^1(C_{\overline{\mathbb{F}}_q}, \mathbb{Q}_\ell)$. Then,*

$$\sum_{x \in \mathrm{Bun}_G(\mathbb{F}_q)} \frac{1}{\# \mathrm{Aut}(x)(\mathbb{F}_q)} = \tau(G) \prod_{p \in C} \frac{1}{\mathrm{vol}(G(\mathscr{O}_p))}$$
$$= \tau(G) q^{(g-1)\dim G} \prod_{i=1}^{\mathrm{rk}\, G} \frac{\prod_{j=1}^{2g}(1-\epsilon_i \alpha_j q^{-d_i})}{(1-\epsilon_i q^{-d_i})(1-\epsilon_i q^{(1-d_i)})}.$$

3 The Cohomology of Bun_G

Our next aim is to recall from [1] the construction of the canonical classes in the cohomology ring of Bun_G and to prove that these generate a free subalgebra over any field. We will then explain how to deduce our main theorem from the purity of the cohomology of Bun_G which will occupy the rest of this article.

3.1 The Subring Generated by the Atiyah–Bott Classes

Fix $\vartheta \in \pi_0(\mathrm{Bun}_G) = \pi_1(G)$. The universal principal G-bundle $\mathscr{P}_{\mathrm{univ}}$ on $\mathrm{Bun}_G^\vartheta \times C$ defines a map $f \colon \mathrm{Bun}_G^\vartheta \times C \to BG$. The characteristic classes of $\mathscr{P}_{\mathrm{univ}}$ are defined as $c_i(\mathscr{P}_{\mathrm{univ}}) := f^\star c_i$ where the c_i are, as in Proposition 2.2.5, the standard generators of the cohomology ring of BG.
Note that the Künneth theorem for stacks can be deduced from the corresponding result for schemes using the spectral sequence computing the cohomology of the stack from the cohomology of an atlas as in Lemma 2.2.2.
We choose a basis $(\gamma_i)_{i=1,\dots,2g}$ of $H^1(C, \overline{\mathbb{Q}}_\ell)$. In the case that C is defined over a finite field k, we choose the γ_i as eigenvectors for the geometric Frobenius of eigenvalue α_i. The Künneth decomposition of $c_i(\mathscr{P}_{\mathrm{univ}})$ is therefore of the form:

$$c_i(\mathscr{P}_{\mathrm{univ}}) =: a_i \otimes 1 + \sum_{j=1}^{2g} b_i^j \otimes \gamma_j + f_i \otimes [\mathrm{pt}].$$

Note that $d_i > 1$, because we assume that G is semisimple. Thus, the f_i are not constant. Of course, these classes depend on ϑ, but we don't want to include this dependence in our notation.

Proposition 3.1.1. *The classes (a_i, b_i^j, f_i) generate a free graded subalgebra of the cohomology ring $H^\star(\mathrm{Bun}_{G,\overline{k}}^\vartheta, \overline{\mathbb{Q}}_\ell)$, i.e., there is an inclusion:*

$$\mathrm{can} \colon \overline{\mathbb{Q}}_\ell[a_1, \dots, a_r] \otimes \bigwedge^{\star}[b_i^j]_{i=1,\dots r, j=1,\dots,2g} \otimes \overline{\mathbb{Q}}_\ell[f_1, \dots, f_r] \hookrightarrow H^\star(\mathrm{Bun}_{G,\overline{k}}^\vartheta, \overline{\mathbb{Q}}_\ell).$$

If k is a finite field, then the classes a_i, b_i^j, f_i are eigenvectors for the action of the arithmetic Frobenius with eigenvalues, $q^{-d_i}, q^{-d_i}\alpha_j, q^{1-d_i}$ respectively.

Proof. Denote by $\mathrm{Can}^\star \subset H^\star(\mathrm{Bun}_G^\vartheta, \overline{\mathbb{Q}}_\ell)$ the subring generated by the classes (a_i, b_i^j, f_i).

Note first that the analog of the theorem holds for $G = \mathbb{G}_m$. In this case, $\mathrm{Bun}_{\mathbb{G}_m}$ is the disjoint union of the stacks $\mathrm{Bun}^d_{\mathbb{G}_m}$ classifying line bundles of degree d. There is the $\mathbb{G}_m$-gerbe $\mathrm{Bun}^d_{\mathbb{G}_m} \to \mathrm{Pic}^d_C$ which is trivial over any field over which C has a rational point, because in this case Pic^d_C is a fine moduli space for line bundles together with a trivialization at a fixed rational point p. Forgetting the trivialization at p corresponds to taking the quotient of Pic by the trivial $\mathbb{G}_m$-action. Thus, $\mathrm{Bun}^d_{\mathbb{G}_m} \cong \mathrm{Pic}^d \times B\mathbb{G}_m$ and the cohomology of this stack is $H^\star(\mathrm{Pic}^d, \overline{\mathbb{Q}}_\ell) \otimes \overline{\mathbb{Q}}_\ell[c_1]$. Here, the first factor is the exterior algebra generated by the Künneth components of the Poincaré bundle.

Let $T \subset G$ be a maximal torus and fix an isomorphism $T \cong \mathbb{G}_m^r$ in order to apply the result for $\mathbb{G}_m$. Then, $X^\star(T)^\vee \cong \mathbb{Z}^r$. Recall furthermore that the G-bundle induced from a T-bundle of degree $\underline{k} \in \mathbb{Z}^r \cong X^\star(T)^\vee$ lies in Bun^ϑ_G, if and only if $\underline{k} \equiv \vartheta \in X^\star(T)^\vee/\Lambda^\vee$. We denote this coset by $\mathbb{Z}^r_\vartheta$.

Write $H^\star(BT_{\overline{k}}, \overline{\mathbb{Q}}_\ell) \cong \overline{\mathbb{Q}}_\ell[x_1, \dots x_r]$ and, for every degree $\underline{k} \in \mathbb{Z}^r$, denote by $A_i, B_i^j \in H^\star(\mathrm{Bun}^{\underline{k}}_T, \overline{\mathbb{Q}}_\ell)$ the Künneth components of the Chern classes of the universal T-bundle. Note that, since $\Lambda^\vee \subset \mathbb{Z}^r$ has finite index, we have the injective map

$$\overline{\mathbb{Q}}_\ell[A_1, \dots, A_r] \otimes \bigwedge^\star [B_i^j]_{i=1,\dots r, j=1,\dots,2g} \otimes \overline{\mathbb{Q}}_\ell[K_1, \dots, K_r] \hookrightarrow \prod_{\underline{k} \in \mathbb{Z}^r_\vartheta} H^\star(\mathrm{Bun}^{\underline{k}}_T, \overline{\mathbb{Q}}_\ell)$$

defined by $K_i \mapsto (k_i)_{\underline{k} \in \mathbb{Z}^r_\vartheta}$ where k_i is considered as an element of $H^0(\mathrm{Bun}^{\underline{k}}_T, \overline{\mathbb{Q}}_\ell) = \overline{\mathbb{Q}}_\ell$.

Recall that the induced map $H^\star(BG_{\overline{k}}, \overline{\mathbb{Q}}_\ell) \to H^\star(BT_{\overline{k}}, \overline{\mathbb{Q}}_\ell) \cong \overline{\mathbb{Q}}_\ell[x_1, \dots, x_{\mathrm{rk}\, G}]$ is given by $c_i \mapsto \sigma_i(x_1, \dots, x_r)$ where σ_i is a homogeneous polynomial of degree d_i. Therefore, we can calculate the image of the canonical classes under the map

$$\begin{aligned} H^\star(\mathrm{Bun}^\vartheta_G, \overline{\mathbb{Q}}_\ell) \otimes H^\star(C, \overline{\mathbb{Q}}_\ell) &\to H^\star(\mathrm{Bun}_T, \overline{\mathbb{Q}}_\ell) \otimes H^\star(C, \overline{\mathbb{Q}}_\ell) \\ &\cong \prod_{\underline{k} \in \mathbb{Z}^r_\vartheta} H^\star(\mathrm{Bun}^{\underline{k}}_T, \overline{\mathbb{Q}}_\ell) \otimes H^\star(C, \overline{\mathbb{Q}}_\ell) \end{aligned}$$

which respects the Künneth decomposition. It is given by

$$c_i(\mathscr{P}_{\mathrm{univ}}) \mapsto \prod_{\underline{k} \in \mathbb{Z}^r_\vartheta} \sigma_i\Big(A_1 \otimes 1 + \sum_{j=1}^{2g} B_1^j \otimes \gamma_j + k_1 \otimes [\mathrm{pt}], \dots\Big).$$

The Künneth decomposition of this class is

$$\begin{aligned}\sigma_i\Big(A_1\otimes 1+\sum_{j=1}^{2g} B_1^j\otimes\gamma_j+k_1\otimes[\mathrm{pt}],\dots\Big)\\ &= \sigma_i(A_1,\dots,A_r)\otimes 1\\ &\quad+\sum_{j=1}^{2g}\Big(\sum_{m=1}^{r}(\partial_m\sigma_i)(A_1,\dots,A_r)\Big)B_m^j\otimes\gamma_j\\ &\quad+\sum_{m=1}^{r}(\partial_m\sigma_i)(A_1,\dots,A_{\mathrm{rk}\,G})k_m\otimes[\mathrm{pt}]\\ &\quad+\sum B_i^jB_{i'}^{j\prime}\cdot P_{j,j'}(A_1,\dots,A_{\mathrm{rk}\,G})\otimes[\mathrm{pt}],\end{aligned}$$

where the $P_{j,j'}$ are some polynomials. In particular, we see that the above map factors through the subring

$$\overline{\mathbb{Q}}_\ell[A_1,\dots,A_r]\otimes\bigwedge^{\star}[B_i^j]_{i=1,\dots r,\ j=1,\dots,2g}\otimes\overline{\mathbb{Q}}_\ell[K_1,\dots,K_r]\hookrightarrow\prod_{\underline{k}\in\mathbb{Z}^r_\vartheta}H^\star(\mathrm{Bun}_T^{\underline{k}},\overline{\mathbb{Q}}_\ell)$$

defined above. We already know that the elements $\sigma_i(A_1,\dots,A_{\mathrm{rk}\,G})$ are algebraically independent in $H^\star(\mathrm{Bun}_{T,\overline{k}},\overline{\mathbb{Q}}_\ell)$. In particular, since the map $\mathbb{A}^{\mathrm{rk}\,G}\to\mathbb{A}^{\mathrm{rk}\,G}\cong(\mathbb{A}^{\mathrm{rk}\,G}/W)$ defined by the polynomials σ_i is generically a Galois covering with Galois group W, we also know that the derivatives $\partial\sigma_i$ are linearly independent. This shows our claim. □

Remark 3.1.2. In the proof above, we have only used the fact that $H^\star(\mathrm{Pic}^0_C,\mathbb{Q}_\ell)\cong\bigwedge^\star H^1(C,\mathbb{Q}_\ell)$. Thus, one might note that the proof shows that for any smooth, projective variety X the analogous classes a_i,b_i^j,f_i^k, where f_i^k are the Künneth components corresponding to a basis of $\mathrm{NS}(X)_{\mathbb{Q}}$, generate a free subalgebra of the cohomology of the moduli stack of principal bundles on X.

In the following, we will denote the graded subring constructed above by $\mathrm{Can}^\star$. Of course, we want to show that $\mathrm{Can}^\star$ is indeed the whole cohomology ring of $\mathrm{Bun}^\vartheta_{G,\overline{k}}$.

Corollary 3.1.3. *Let k be a finite field and let $G_{/k}$ be a semisimple group. If $H^\star(\mathrm{Bun}^\vartheta_{G,\overline{k}},\overline{\mathbb{Q}}_\ell)$ is generated by the canonical classes for all ϑ, then the Tamagawa number $\tau(G)$ satisfies $\tau(G)=\dim H^0(\mathrm{Bun}_G,\overline{\mathbb{Q}}_\ell)=\#\pi_0(\mathrm{Bun}_G)$. Conversely, if the cohomology of Bun_G is pure and the Tamagawa number fulfills $\tau(G)=\#\pi_0(\mathrm{Bun}_G)$, then $H^\star(\mathrm{Bun}_G,\overline{\mathbb{Q}}_\ell)=\mathrm{Can}^\star$.*

Proof. For the graded ring Can^i generated by the canonical classes, we know that

$$\sum_{i=0}^\infty(-1)^i\,\mathrm{tr}(\mathrm{Frob},\mathrm{Can}^i)=\frac{\prod_{i=1}^r\prod_{j=1}^{2g}(1-\epsilon_i\alpha_jq^{-d_i})}{\prod_{i=1}^r(1-\epsilon_iq^{-d_i})(1-\epsilon_iq^{1-d_i})}.$$

Comparing this with Siegel's formula, we get the first claim.
Furthermore we know that the Zeta function of Bun_G converges and is equal to

$$\begin{aligned} Z(\mathrm{Bun}_G, t) &= \exp\Big(\sum_{i=1}^{\infty} \#\mathrm{Bun}_G(\mathbb{F}_{q^n})\frac{t^i}{i}\Big) \\ &= \prod_{i=0}^{\infty} \det\Big(1 - \mathrm{Frob}\cdot q^{\dim(\mathrm{Bun}_G)} \cdot t, H^i(\mathrm{Bun}_G, \overline{\mathbb{Q}}_\ell)\Big)^{(-1)^{i+1}}. \end{aligned}$$

Now, since such a product expansion of an analytic function is unique and the eigenvalues of Frob on H^i have absolute value $q^{i/2}$, there can be no cancellations. Thus, the Poincaré series of the cohomology ring can be read off the Zeta function. □

3.2 The Main Results on Moduli Spaces of Flagged Principal Bundles

Let $\underline{x} = (x_i)_{i=1,\dots,b}$ be a finite set of distinct k-rational points of C, and let $\underline{P} = (P_i)_{i=1,\dots,b}$ be a tuple of parabolic subgroups of G. A *principal G-bundle with a flagging of type* $(\underline{x}, \underline{P})$ is a tuple $(\mathscr{P}, \underline{s})$ that consists of a principal G-bundle $\mathscr{P}$ on C and a tuple $\underline{s} = (s_1, ..., s_b)$ of sections $s_i \colon \{x_i\} \to (\mathscr{P} \times_C \{x_i\})/P_i$, i.e., s_i is a reduction of the structure group of $\mathscr{P} \times_C \{x_i\}$ to P_i, $i = 1, ..., b$.

Remark 3.2.1. For $G = \mathrm{GL}_r(k)$, parabolic subgroups correspond to flags of quotients of k^r, so that a flagged principal $\mathrm{GL}_r(k)$-bundle may be identified with a vector bundle $\mathscr{E}$ together with flags of quotients $\mathscr{E}_{x_i} \twoheadrightarrow V_{j,i}$, $j = 1, ..., t_i$, $i = 1, ..., b$, of the fibers of $\mathscr{E}$ at x_i, $i = 1, ..., b$. (A "flag of quotients" means of course that $K_{1,i} \subsetneq \cdots \subsetneq K_{t_i,i}$, $K_{j,i} := \ker(\mathscr{E}_{x_i} \twoheadrightarrow V_{j,i})$, $j = 1, ..., t_i$, $i = 1, ..., b$.) These objects were introduced by Mehta and Seshadri [31] and called *quasi-parabolic vector bundles*. We had to chose a different name, because the notion of a *parabolic principal bundle* has been used differently in [2]. The same objects that we are looking at have also been considered in [9] and [43].

Lemma 3.2.2. *Fix a type $(\underline{x}, \underline{P})$ as in the definition.*
i) *The principal G-bundles with a flagging of type $(\underline{x}, \underline{P})$ form the smooth algebraic stack* $\mathrm{Bun}_{G,\underline{x},\underline{P}}$.
ii) *The forgetful map* $\mathrm{Bun}_{G,\underline{x},\underline{P}} \to \mathrm{Bun}_G$ *is a locally trivial bundle whose fibers are isomorphic to* $\prod_{i=1}^{s}(G/P_i)$.
iii) *The cohomology algebra* $H^\star(\mathrm{Bun}_{G,\underline{x},\underline{P}}, \overline{\mathbb{Q}}_\ell)$ *is a free module over* $H^\star(\mathrm{Bun}_G, \overline{\mathbb{Q}}_\ell)$ *with a basis of pure cohomology classes. The same holds for all open substacks of* Bun_G *and their preimages in* $\mathrm{Bun}_{G,\underline{x},\underline{P}}$.

Proof. The first parts are easy, because for a G-bundle $\mathscr{P} \to T \times C$ the space $\prod_i (\mathscr{P}|_{T\times x_i})/P_i \to T$ parameterizes flaggings of $\mathscr{P}$ at $T \times \underline{x}$. This is a $\prod_{i=1}^{s}(G/P_i)$ bundle over T. The last part follows from the second by the theorem of Leray–Hirsch: the flagging of the universal bundle at x_i defines a P_i-bundle over $\mathrm{Bun}_{G,\underline{x},\underline{P}}$ and thus a map $\mathrm{Bun}_{G,\underline{x},\underline{P}} \to BP_i$. But the map $G/P_i \to BP_i$ induces a surjection on cohomology, and thus the pull back of the universal classes in $H^\star(BP_i, \overline{\mathbb{Q}}_\ell)$ to $H^\star(\mathrm{Bun}_{G,\underline{x}}, \overline{\mathbb{Q}}_\ell)$ generate the cohomology of all the fibers of $\mathrm{Bun}_{G,\underline{x}} \to \mathrm{Bun}_G$. ☐

In Section 4, we will introduce a notion of $\underline{a}$-stability for flagged principal bundles depending on some parameter $\underline{a}$. As in the case of vector bundles, we will define a coprimality condition for $\underline{a}$ (see 4.2.1) as well as some admissibility condition (following Remark 4.1.5).

In $\mathrm{Bun}_{G,\underline{x},\underline{P}}$ there are open substacks $\mathrm{Bun}_{G,\underline{x},\underline{P}}^{\underline{a}\text{-(s)s}}$ of $\underline{a}$-(semi)stable flagged principal G-bundles of type $(\underline{x},\underline{P})$. Our main results on the coarse moduli spaces of these substacks are collected in the following theorem.

Theorem 3.2.3. i) *For any type* $(\underline{x},\underline{P})$ *and any admissible stability parameter* $\underline{a}$*, there exists a projective coarse moduli space* $\mathscr{M}(\underline{x},\underline{P})^{\underline{a}\text{-ss}}$ *for* $\underline{a}$*-semistable flagged principal* G*-bundles of type* $(\underline{x},\underline{P})$*.*

ii) *If* $\underline{a}$ *is of coprime type, then the notions of* $\underline{a}$*-semi stability and* $\underline{a}$*-stability coincide. In this case,* $\mathrm{Bun}_{G,\underline{x},\underline{P}}^{\underline{a}\text{-s}}$ *is a proper, smooth quotient-stack with finite stabilizer groups.*

iii) *For any substack* $U \subset \mathrm{Bun}_G$ *of finite type and any* $i > 0$*, there exist* $s > 0$*, a type* $(\underline{x},\underline{P})$*, and an admissible stability parameter* $\underline{a}$ *of coprime type, such that* U *lies in the image of the map* $\mathrm{Bun}_{G,\underline{x},\underline{P}}^{\underline{a}\text{-s}} \to \mathrm{Bun}_G$ *and such that the subset of* $\underline{a}$*-unstable bundles is of codimension* $> i$ *in* $\mathrm{Bun}_{G,\underline{x},\underline{P}}$*.*

The proof of this theorem takes up the largest part of this article. We will prove the existence of the coarse moduli spaces in Section 5. The projectivity then follows from our semistable reduction theorem 4.4.1. The last two parts of the theorem are much easier. We will prove them in Section 4.

Remark 3.2.4. For simplicity, we have stated Theorem 3.2.3 only for curves defined over a field. In order to prove our base change theorem, we will need the result in the case that C is a smooth, projective family of curves with geometrically reduced, connected fibers, defined over an integral ring R, finitely generated over $\mathbb{Z}$, and G a semisimple Chevalley group over R.

Seshadri proved in [39] (Theorem 4, p. 269) that GIT-quotients can be constructed for families over R. Further, the parameter spaces constructed in Section 5 are given by quot schemes which exist over base schemes, and, in Section 5.6, we finally need a Poincaré bundle on the relative Picard scheme. A Poincaré bundle exists, if the family $C \longrightarrow \mathrm{Spec}(R)$ has a section. This certainly holds after an étale extension of R. Hence, the first assertion still holds after an étale extension of R.

Except for the properness assertion for the stack of stable flagged principal bundles which is Lemma 3.3.1, the last two parts of the theorem carry over to this situation without modification.

We will come back to the issue of the base ring in Remarks 5.2.4, 5.3.3, and 5.5.4.

Before we proceed with the proof of the theorem, we want to deduce our main application.

3.3 Purity of $H^\star(\mathrm{Bun}_G)$

Assume that k is a finite field. Since all open substacks of finite type of Bun_G can be written as $[X/\mathrm{GL}_N]$ where X is a smooth variety, we know that the eigenvalues λ_i of the (arithmetic) Frobenius on $H^i(\mathrm{Bun}_G, \overline{\mathbb{Q}}_\ell)$ satisfy $|\lambda_i| \leq q^{-\frac{i}{2}}$ [8]. To prove equality, i.e., to prove that the cohomology is pure, we cannot rely on such a general argument. But, using the results on coarse moduli spaces, we can show that for all i the cohomology $H^i(\mathrm{Bun}_G, \overline{\mathbb{Q}}_\ell)$ occurs as a direct summand in the i-th cohomology of a projective variety, parameterizing stable flagged principal bundles.

Lemma 3.3.1. *Assume that R is a field or a discrete valuation ring with quotient field K. Let $G_{/R}$ be a reductive group, acting on the projective scheme $\overline{X}_R$ and $\mathscr{L}$ a G-linearized ample line bundle on $\overline{X}_R$, such that all points of $X := \overline{X}^{\mathrm{ss}}_{\mathscr{L}}$ are stable with respect to the chosen linearization. Then, the quotient stack $[X/G]$ is separated and the map $[X/G] \to X/\!\!/G$ is proper.*

Proof. If R is a field, we can apply GIT ([32] Corollary 2.5), saying that the map $G \times X \to X \times X$ is proper. Therefore, the diagonal $[X/G] \to [X/G] \times [X/G]$ is universally closed, i.e., $[X/G]$ is separated.

We claim that we may prove the separatednedness of the map $[X/G] \to X/\!\!/G$ over a discrete valuation ring R in the same manner. To show the lifting criterion for properness for the group action, we assume that we are given $x_1, x_2 \in X(R)$ and $g \in G(K)$, such that $g.x_1 = x_2$. We have to show that $g \in G(R)$. We may (after possibly replacing R by a finite extension as in [32], Appendix to Chapter 2.A) apply the Iwahori decomposition to write $g = g_0 z g_0'$ with $g_0, g_0' \in G(R)$ and $z \in T(K)$ for a maximal torus $T \subset G$. Thus, we have reduced the problem to the case that $g = z \in T(K)$. Choose a local parameter $\pi \in R$. Multiplying with an element of $T(R)$, we may further assume that there is a one-parameter subgroup $\lambda\colon \mathbb{G}_m \to T$, such that $z = \lambda(\pi)$. Assume that λ is non-trivial. Now, embed $\overline{X}_R \subset \mathbb{P}(V)$ into a projective space and decompose $V = \sum_{i\in\mathbb{Z}} V_i$ into the eigenspaces of λ. Write $x_1 = \sum_{i\in\mathbb{Z}} v_i$ and $x_2 = \sum_{i\in\mathbb{Z}} w_i$ as sums of eigenvectors for λ. Since the reduction $\overline{x}_1$ of $x_1 \mod \pi$ is stable, there must be indices $i_- < 0 < i_+$ with $\overline{v}_{i_-} \neq 0 \neq \overline{v}_{i_+}$. The analogous condition holds for $\overline{x}_2$. But, one readily checks that $x_2 = z.x_1$ implies $\overline{w}_i = 0$, for $i > 0$, a contradiction.

Now, for algebraically closed fields K, the map $[X/G] \to X/\!\!/G$ induces a bijection on isomorphism classes of K-points. Thus, since we already know separatedness, it is sufficient to show that given a discrete valuation ring R and a point $\overline{x} \in X/\!\!/G(R)$, then we can find an extension R' of R, such that $\overline{x}$ lifts to a point $x \in X(R')$ and thus to a point in $[X/G]$. Let K be the quotient field of R, $\eta \in X$ a point lying over the generic point of $\overline{x}$. Then, the closure of $G \times \eta \subset X$ is a G-invariant subset. Since $X/\!\!/G$ is a good quotient, its image is closed and contains $\overline{x}$. Thus, the orbit of η specializes to a point lying over the closed point of $\overline{x}$, and we can find $x \in X(R')$ as claimed. $\square$

Corollary 3.3.2. *Assume that C is a smooth projective curve, defined over the finite field k. If $\underline{a}$ is of coprime type, then $H^\star(\mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}}, \overline{\mathbb{Q}}_\ell)$ is pure.*

Proof. The stack $\mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}}$ of $\underline{a}$-stable flagged principal G-bundles of type $(\underline{x}, \underline{P})$ is a smooth quotient stack. Therefore, its i-th cohomology is of weight $\geq i$. This is proved in [8], Theorem 5.21. (Observe the different conventions for the Frobenius map.) Furthemore, by the definition of stability, all automorphism groups of stable parabolic bundles are finite. In particular, by the preceding lemma, the map $p\colon \mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}} \to \mathscr{M}(\underline{x}, \underline{P})^{\underline{a}\text{-s}}$ is proper. In order to prove that $Rp_\star\mathbb{Q}_\ell \cong \mathbb{Q}_\ell$, it is therefore sufficient to compare the stalks of these sheaves ([34], Theorem 1.3). But the fibers are quotients of $\mathrm{Spec}(K)$ by finite group schemes. Thus, for rational coefficients, the higher cohomology of the fibers vanishes. In particular, p induces an isomorphism on cohomology. Since the scheme $\mathscr{M}(\underline{x}, \underline{P})^{\underline{a}\text{-s}}$ is proper (Theorem 3.2.3), its i-th cohomology is of weight $\leq i$, by Deligne's theorem ([12], Théorème I), $\square$

Remark 3.3.3. i) So far, we have treated the moduli spaces only over algebraically closed fields. Of course, they will be defined over a finite extension of $\mathbb{F}_q$. (In fact, as the construction of the moduli spaces will reveal, they will be defined over the same field as the points in the tuple $\underline{x}$.) If we replace $\mathbb{F}_q$ by a finite extension, the new Frobenius is a power of the original Frobenius. The purity statement is obviously not affected, because it concerns only the absolute values of the eigenvalues of the Frobenius map.
ii) The moduli space $\mathscr{M}(\underline{x}, \underline{P})^{\underline{a}\text{-s}}$ will, in general, have finite quotient singularities. Therefore, we could obtain both estimates for the weights from the coarse moduli space.

Corollary 3.3.4. *Suppose R is of finite type over $\mathbb{Z}$, regular, and of dimension at most 1, and let $C_{/R}$ be a smooth projective curve and G a split semisimple group scheme over R. Then, the cohomology of $\mathrm{Bun}_G \to \mathrm{Spec}(R)$ is locally constant over $\mathrm{Spec}(R)$.*

Proof. By Theorem 3.2.3, iii), we know that, for fixed i, the i-th cohomology sheaf of Bun_G is a direct summand of the corresponding sheaf of $\mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}}$ for suitable type $(\underline{x}, \underline{P})$ and suitable stability parameter $\underline{a}$. Further, by Lemma 3.3.1, the map $p\colon \mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}} \to \mathscr{M}(\underline{x}, \underline{P})^{\underline{a}\text{-s}}$ is proper. Since the coarse moduli space is proper as well, we can again apply Olsson's base change theorem ([34], Theorem 1.3) to the proper map $\pi : \mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}} \to \mathscr{M}(\underline{x}, \underline{P})^{\underline{a}\text{-s}} \to \mathrm{Spec}(R)$. In particular, the fibers of $\mathbb{R}\pi_\star\mathbb{Q}_\ell$ compute the cohomology of the fibers of π.
Moreover, the stack $\mathscr{X} := \mathrm{Bun}^{\underline{a}\text{-s}}_{G,\underline{x},\underline{P}}$ is smooth. Thus, we may use local acyclicity of smooth maps as in [11], Chapitre V. To see that this holds for stacks, let us recall the argument. We may suppose that the base $S = \mathrm{Spec}(R)$ is strictly

henselian. Denote by $\overline{\eta}$ the spectrum of an algebraic closure of the generic point of S and let s denote the special point of S. We have a cartesian diagram

$$\begin{array}{ccccc} \mathscr{X}_{\overline{\eta}} & \xrightarrow{\epsilon'} & \mathscr{X} & \xleftarrow{i'} & \mathscr{X}_s \\ \downarrow & & \downarrow f & & \downarrow \\ \overline{\eta} & \xrightarrow{\epsilon} & S & \xleftarrow{i} & \{s\}. \end{array}$$

Now, $\mathbb{R}\epsilon'_\star\mathbb{Q}_\ell \cong f^\star\mathbb{R}\epsilon_\star\mathbb{Q}_\ell$, because this holds for any smooth covering $U \to \mathscr{X}$ and $i'^*\mathbb{R}\epsilon_\star\mathbb{Q}_\ell = \mathbb{Q}_\ell$. Thus, using the above calculation and proper base change for the last equality, we find:

$$H^\star(\mathscr{X}_{\overline{\eta}}, \mathbb{Q}_\ell) \cong H^\star(\mathscr{X}, \mathbb{R}\epsilon'_\star\mathbb{Q}_\ell) \cong H^\star(\mathscr{X}_s, \mathbb{Q}_\ell).$$

This settles the claim. □

We may now derive our main result.

Theorem 3.3.5. *Assume that C is a curve over the field k. Then, the cohomology of* Bun_G *is freely generated by the canonical classes, i.e.,*

$$H^\star\big(\mathrm{Bun}^{\vartheta}_{G,\overline{k}}, \overline{\mathbb{Q}}_\ell\big) = \overline{\mathbb{Q}}_\ell[a_1, \ldots, a_r] \otimes \bigwedge^{\star}[b_i^j]_{i=1,\ldots,r, j=1,\ldots,2g} \otimes \overline{\mathbb{Q}}_\ell[f_1, \ldots, f_r].$$

Proof. First method. One can deduce the result from the theorem of Atiyah and Bott. By the base change corollary above, knowing the theorem for $k = \mathbb{C}$ implies the claim over an arbitrary algebraically closed field. For $k = \mathbb{C}$ Atiyah and Bott proved the result. Namely they constructed a continuous atlas $X \to \mathrm{Bun}_G$, where X is contractible and Bun_G is the quotient of X by the action of an infinite dimensional group $\mathscr{G}$. In the article of Atiyah and Bott the equivariant cohomology of X with respect to this group action is computed. However, the spectral sequence computing equivariant cohomology from the cohomology of $\mathscr{G}$ coincides with the sequence computing the cohomology of Bun_G from the atlas $X \to \mathrm{Bun}_G$.

Second method. By the base change corollary 3.3.4, it is sufficient to prove the claim in the case that C is defined over a finite field k. We have just seen (Corollary 3.3.2) that in this case the cohomology of Bun_G is pure. Furthermore, Harder proved [18] that $\tau(G) = 1$ for semisimple simply connected groups and Ono showed how to deduce $\tau(G) = \#\pi_1(G)$ for arbitrary semisimple groups (see [8], §6). Thus, we can apply Corollary 3.1.3 to Siegel's formula and Behrend's trace formula. □

Remark 3.3.6. For $G = \mathrm{SL}_n(k)$ (or $G = \mathrm{GL}_n(k)$), one can use Beauville's trick [3] which shows that the cohomology of $\mathrm{Bun}^{\underline{a}\text{-s}}_{\mathrm{SL}_n,\underline{x},\underline{P}}$ is generated by the classes constructed in Remark 3.2.2. This gives a direct proof of the theorem.

4 Semistability for Flagged Principal Bundles

In this section, we introduce the parameter dependent notion of semistability for flagged principal bundles. After discussing its basic features, including the important fact that any principal bundle can be turned into a stable flagged principal bundle for a suitable type and a suitable stability parameter, we apply Behrend's formalism of complementary polyhedra to derive the Harder–Narasimhan reduction for semistable flagged principal bundles. We conclude with a proof of the semistable reduction theorem for flagged principal bundles, generalizing the arguments from [22] and [23].

4.1 Definition of Semistability

We want to define a notion of semistability for flagged principal bundles. For an algebraic group P let us denote by $X^\star(P) := \mathrm{Hom}(P, \mathbb{G}_m)$ the group of characters and by $X^\star(P)^\vee_{\mathbb{Q}} := \mathrm{Hom}(X^\star(P), \mathbb{Q})$ the rational cocharacters. The notion of semistability will depend on parameters a_i varying over the sets

$$X^\star(P_i)^\vee_{\mathbb{Q},+} := \left\{ a \in X^\star(P_i)^\vee_{\mathbb{Q}} \;\middle|\; \begin{array}{l} \text{for all parabolic subgroups } P' \supset P_i \\ a(\det_{P'} \otimes \det_{P_i}^{-1}) < 0 \end{array} \right\},$$

$i = 1, ..., b$. (Since $\mathrm{Bun}_{G,\underline{x},\underline{P}} \to \mathrm{Bun}_G$ is a locally trivial fibration with fiber $\prod_{i=1}^s G/P_i$, we see that the Picard group of $\mathrm{Bun}_{G,\underline{x},\underline{P}}$ is a free $\mathbb{Z}$-module generated by $\mathrm{Pic}(\mathrm{Bun}_G) \cong \mathbb{Z}$ and $\prod_{i=1}^s X^\star(P_i)$. Therefore the notion of semistability should depend on an element in $X^\star(P_i)^+$. Since this has a canonical basis, the dual appears in our definition.) To state this in terms closer to Geometric Invariant Theory, note that the pairing of characters and one-parameter subgroups of a parabolic subgroup of G is invariant under conjugation. Therefore, conjugacy classes of rational one-parameter subgroups of P_i are given by $X^\star(P_i)^\vee_{\mathbb{Q}}$, $i = 1, ..., b$. A one-parameter subgroup $\lambda\colon \mathbb{G}_m \to G$ defines the parabolic subgroup

$$P(\lambda) := P_G(\lambda) = \Big\{ g \in G \,\Big|\, \lim_{z \to 0} \lambda(z) g \lambda(z)^{-1} \text{ exists in } G \Big\}.$$

For later purposes, we also introduce

$$Q_G(\lambda) := P_G(-\lambda) = \Big\{ g \in G \,\Big|\, \lim_{z \to \infty} \lambda(z) g \lambda(z)^{-1} \text{ exists in } G \Big\}.$$

Example 4.1.1. Any one-parameter subgroup $\lambda\colon \mathbb{G}_m(k) \longrightarrow \mathrm{GL}(V)$ defines a set of weights $\gamma_1 < \cdots < \gamma_{t+1}$ and a decomposition

$$V = \bigoplus_{l=1}^{t+1} V^l \text{ with } V^l := \Big\{ v \in V \,\Big|\, \lambda(z)(v) = z^{\gamma_l} \cdot v,\ \forall z \in \mathbb{G}_m(k) \Big\},\ l = 1, ..., t{+}1,$$

into eigenspaces. We derive the flag

$$V_\bullet(\lambda) : \{0\} \subsetneq V_1 := V^1 \subsetneq V_2 := V^1 \oplus V^2 \subsetneq \cdots \subsetneq V_t := V^1 \oplus \cdots \oplus V^t \subsetneq V.$$

Note that the group $Q_{\mathrm{GL}(V)}(\lambda)$ is the stabilizer of the flag $V_\bullet(\lambda)$. As an additional datum, we define the tuple $\beta_\bullet(\lambda) = (\beta_1, ..., \beta_t)$ with $\beta_l := (\gamma_{l+1} - \gamma_l)/\dim(V)$, $l = 1, ..., t$. The pair $(V_\bullet(\lambda), \beta_\bullet(\lambda))$ is the *weighted flag of* λ.

Since $P(\lambda) = P(n\lambda)$ for all $n \in \mathbb{N}$, the group $P(\lambda)$ is also well defined for rational one-parameter subgroups, and it only depends on the conjugacy class of λ in $P(\lambda)$. Finally, writing G as a product of root groups, we see that $\lambda \in X_\star(P_i)_\mathbb{Q}$ defines an element $\lambda \in X^\star(P_i)^\vee_{\mathbb{Q},+}$, if and only if $P_i = P(\lambda)$. It will often be convenient for us to view $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$ as a rational one-parameter subgroup of G which we will denote by the same symbol.

Remark 4.1.2. i) Let $(\mathscr{P}, \underline{s})$ be a flagged principal G-bundle and $\mathscr{P}_{x_i,P_i}$ the P_i-torsor over x_i defined by s_i, $i = 1, ..., b$. Denote further $P_{s_i} := \mathrm{Aut}_{P_i}(\mathscr{P}_{x_i,P_i}) \subset \mathrm{Aut}_G(\mathscr{P}_{x_i})$ the corresponding parabolic subgroup. Any (P_i-equivariant) trivialization $\mathscr{P}_{x_i,P_i} \cong P_i$ defines an isomorphism $P_{s_i} \cong P_i$. This isomorphism is canonical up to inner automorphisms of P_i, so that we obtain canonical isomorphisms $X^\star(P_i)_\mathbb{Q} \cong X^\star(P_{s_i})_\mathbb{Q}$ and $X^\star(P_i)^\vee_{\mathbb{Q},+} \cong X^\star(P_{s_i})^\vee_{\mathbb{Q},+}$, $i = 1, ..., b$. Given $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$ we will denote the corresponding element in $X^\star(P_{s_i})^\vee_{\mathbb{Q},+}$ by a_{s_i}. The "one-parameter subgroup" a_{s_i} is well-defined only up to conjugation in P_{s_i}. If we choose a maximal torus $T \subset P_{s_i}$, we may assume that a_{s_i} is a one-parameter subgroup of T. As such it is well-defined.
ii) Likewise, if a parabolic subgroup Q of G, a character χ of Q, and a reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to Q are given, then we get in each point x_i a parabolic subgroup Q_i in $\mathrm{Aut}(\mathscr{P}_{x_i})$ and a character χ_{s_i} of that parabolic subgroup, $i = 1, ..., b$.
iii) Any two parabolic subgroups P and Q of G share a maximal torus, and all common maximal tori are conjugate in $Q \cap P$. Let $Q_i \subset \mathrm{Aut}(\mathscr{P}_{x_i})$ be a parabolic subgroup, $i = 1, ..., b$. By our previous remarks, we may assume that a_{s_i} is a subgroup of $Q_i \cap P_{s_i}$. Then, for any i and any character $\chi_i \in X^\star(Q_i)$, the value of the pairing $\langle \chi_i, a_{s_i} \rangle$ is well-defined.

These remarks also show the following.

Lemma 4.1.3. *Let $Q, P \subset G$ be parabolic subgroups, $a \in X^\star(P)^\vee_{\mathbb{Q},+}$, and $\chi \in X^\star(Q)$ a dominant character. Denote by ${}^g\chi = \chi(g^{-1} \cdot \_ \cdot g)$ the corresponding character of gQg^{-1}. Then, the value of the function*

$$\begin{aligned} G &\longrightarrow \mathbb{Q} \\ g &\longmapsto \langle {}^g\chi, a \rangle \end{aligned}$$

at an element of G depends only on the image of that element in $Q\backslash G/P$.

Example 4.1.4. Using the notations of the above lemma, assume that $P = B$ is a Borel subgroup and assume that Q contains B. Choose a maximal torus $T \subset B$, denote by Δ_P and Δ_Q the roots of P and Q, respectively, and by W and W_Q the Weyl groups of G and $Q/R_u(Q)$, respectively. Then, the double coset $Q\backslash G/P$ is in bijection to $W_Q\backslash W$ and, by Bruhat decomposition, we know that $QwP/P \subset G/P$ lies in the closure of $Qw'P/P$ only if all roots of wQw^{-1} which do not lie in Δ_P are contained in $\Delta_{w'Qw'^{-1}}$. Now, since $a \in X^\star(P)^\vee_{\mathbb{Q},+}$,

we know that $\langle\alpha, a\rangle < 0$ occurs precisely for the roots $\alpha \notin \Delta_P$. Thus, we find $\langle{}^{w}\chi, a\rangle \geq \langle{}^{w'}\chi, a\rangle$, whenever QwP lies in the closure of $Qw'P$ and equality implies that the double cosets coincide.
In particular the largest value of $\langle{}^{w}\chi, a\rangle$ is obtained for $w = 1$ and the most negative one for the longest element of W.

Fix $\underline{a} \in \prod_{i=1}^{b} X^\star(P_i)^\vee_{\mathbb{Q},+}$. Using Remark 4.1.2 and Lemma 4.1.3, we define the *$\underline{a}$-parabolic degree* (*of the reduction $\mathscr{P}_Q$ of $\mathscr{P}$*) as the function

$$\begin{aligned} \underline{\underline{a}\text{-deg}(\mathscr{P}_Q)} : X^\star(Q) &\longrightarrow \mathbb{Q} \\ \chi &\longmapsto \deg\big(\mathscr{P}_Q(\chi)\big) + \sum_{i=1}^{b} \langle \chi_{s_i}, a_{s_i}\rangle. \end{aligned}$$

(As usual, $\mathscr{P}_Q(\chi)$ is the line bundle on C that is associated with the principal Q-bundle $\mathscr{P}_Q$ and the character $\chi\colon Q \longrightarrow \mathbb{G}_m(k)$.) We write $\underline{a}\text{-deg}(\mathscr{P}_Q) := \underline{\underline{a}\text{-deg}(\mathscr{P}_Q)}(\det_Q)$ where $\det_Q$ is the character defined by the determinant of the adjoint representation of Q.
A flagged principal G-bundle $(\mathscr{P}, \underline{s})$ is called *$\underline{a}$-(semi)stable*, if for any parabolic subgroup $Q \subset G$ and any reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to Q, the condition

$$\underline{a}\text{-deg}(\mathscr{P}_Q)(\leq)0$$

is verified. Here the standard notation $(\leq)$ means that for stable bundles we require a strict inequality, whereas for semistable bundles $\leq$ is allowed.
The *$\underline{a}$-parabolic degree of instability of* $(\mathscr{P}, \underline{s})$ is set to be

$$\begin{aligned} \text{ideg}_{\underline{a}}(\mathscr{P}, \underline{s}) \quad := \quad \max\Big\{ \underline{a}\text{-deg}(\mathscr{P}_Q) \,\big|\, & Q \subset G \text{ a parabolic subgroup} \\ & \text{and } \mathscr{P}_Q \text{ a reduction of } \mathscr{P} \text{ to } Q \Big\}. \end{aligned}$$

Remark 4.1.5. i) Let Q be a maximal parabolic subgroup of G. Then, all dominant characters on Q are positive rational multiples of the corresponding *fundamental weight*. Thus, they are also positive rational multiples of the character $\det_Q$. If Q is an arbitrary parabolic subgroup and χ is a dominant character on it, then one finds maximal parabolic subgroups $Q_1, ..., Q_T$ that contain it and such that χ is a positive rational linear combination of the characters $\det_{Q_1}$,...,$\det_{Q_T}$ (viewed as characters of Q). Therefore, a flagged principal G-bundle $(\mathscr{P}, \underline{s})$ is $\underline{a}$-semistable, if and only if for any parabolic subgroup Q, any reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to Q, and any dominant character $\chi \in X^\star(Q)$, we have $\underline{\underline{a}\text{-deg}(\mathscr{P}_Q)}(\chi) \leq 0$. Or, equivalently, we may use anti-dominant characters χ and require $\underline{\underline{a}\text{-deg}(\mathscr{P}_Q)}(\chi) \geq 0$. (We have used the version with dominant characters, because this allows us to adapt Behrend's existence proof of the canonical reduction ([4], [6]) more easily. For our GIT computations below, the formulation with anti-dominant characters seems better suited.)
ii) From our observations in i), we also infer that it suffices to test semistability for maximal parabolic subgroups.

iii) The $\underline{a}$-parabolic degree of instability is finite, because the degree of instability is finite and the values of $\langle \chi_{s_i}, a_{s_i}\rangle$, $i = 1, ..., b$, are bounded for every fixed $\underline{a}$, and only finitely many χ occur.

An element $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$ is called *admissible*, if for some maximal torus $T \subset P_i$, such that a_i factors through T, we have $|\langle \alpha, a_i\rangle| < \frac{1}{2}$ for all roots α. Note that this does not depend on the choice of T, because all maximal tori are conjugate over k and conjugation permutes the roots. The stability parameter $\underline{a}$ is called *admissible*, if a_i is admissible for $i = 1, ..., b$.

4.2 General Remarks on Semistability

As in the case of vector bundles, the notions of $\underline{a}$-semistability and $\underline{a}$-stability will coincide, if $\underline{a}$ satisfies some coprimality condition. In the following lemma, we will also allow real stability parameters $\underline{a} \in \bigoplus_{i=1}^b X^\star(P_i)^\vee_{\mathbb{R}}$ in order to define a nice chamber decomposition. Clearly, $\underline{a}$-(semi)stability may also be defined for such parameters.

Lemma 4.2.1. *Fix the type $(\underline{x}, \underline{P})$. For every parabolic subgroup $Q \in G$ and every $d \in \mathbb{Z}$, we introduce the* wall

$$W_{Q,d} := \left\{ \underline{a} \in \bigoplus_{i=1}^b X^\star(P_i)^\vee_{\mathbb{R}} \mid \sum_{i=1}^b \langle \det_Q, a_i\rangle = d \right\}.$$

Then, the following properties are satisfied:
i) *For every bounded subset $A \subset X^\star(P_i)^\vee_{\mathbb{R}}$, there are only finitely many walls $W_{Q,d}$ with $W_{Q,d} \cap A \neq \varnothing$.*
ii) *If one of the groups P_i is a Borel subgroup, then $W_{Q,d}$ is for all parabolic subgroups Q and all integers d a proper subset of codimension 1 or empty.*
iii) *If*

$$\underline{a} \notin \bigcup_{Q \subset G \text{ parabolic},\ d \in \mathbb{Z}} W_{Q,d},$$

then every $\underline{a}$-semistable bundle is $\underline{a}$-stable.
iv) *If the stability parameters $\underline{a}$ and $\underline{a}'$ lie in the same connected component of*

$$\bigoplus_{i=1}^b X^\star(P_i)^\vee_{\mathbb{R}} \setminus \bigcup_{Q \subset G \text{ parabolic},\ d \in \mathbb{Z}} W_{Q,d},$$

then the notions of $\underline{a}$-(semi)stability and $\underline{a}'$-(semi)stability coincide.
v) *Let $\mathscr{C}$ be a connected component of $\bigoplus_{i=1}^b X^\star(P_i)^\vee_{\mathbb{R}} \setminus \bigcup_{Q \subset G \text{ parabolic},\ d \in \mathbb{Z}} W_{Q,d}$. If $\underline{a} \in \mathscr{C}$ and $\underline{a}' \in \overline{\mathscr{C}}$, then every $\underline{a}'$-stable bundle is $\underline{a}$-stable and every $\underline{a}$-semistable bundle is $\underline{a}'$-semistable.*

A stability parameter $\underline{a}$ satisfying the condition stated in iii) of the lemma is said to be *of coprime type*.

Proof. Let $\mathfrak{c}$ be a conjugacy class of parabolic subgroups in G and $Q_{\mathfrak{c}}$ a representative of $\mathfrak{c}$. For a parabolic subgroup Q in the class $\mathfrak{c}$ and $i \in \{1, ..., b\}$, the number $\langle \det_Q, a_i \rangle$ depends only on the class of Q in $Q_{\mathfrak{c}} \backslash G/P_i$. This was shown in Lemma 4.1.3. Since there are only finitely many conjugacy classes of parabolic subgroups and any set of the form $Q\backslash G/P$, P, Q parabolic subgroups of G, is finite, there are only finitely many functions of the form

$$\underline{a} \longmapsto \sum_{i=1}^{b} \langle \det_Q, a_i \rangle$$

on $\bigoplus_{i=1}^b X^\star(P_i)^\vee_{\mathbb{R}}$, and any bounded set A is "hit" by only finitely many walls. The second part is easy, because, for a Borel subgroup, one has $X^\star(B) = X^\star(T)$, so that $\langle \det_Q, . \rangle$ cannot vanish identically on $X^\star(B)^\vee_{\mathbb{R}}$.
For a properly semistable flagged principal G-bundle $(\mathscr{P}, \underline{s})$, there are a parabolic subgroup Q and a reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to Q, such that $\sum_{i=1}^b \langle \det_Q, a_i \rangle = -\deg(\mathscr{P}_Q) \in \mathbb{Z}$. This immediately yields iii) and also proves the last two statements. □

Proposition 4.2.2. *Fix a connected component* Bun_G^ϑ *of* Bun_G *and a Borel subgroup* $B \subset G$. *Then, for all* $h \in \mathbb{Z}$, *there exists a number* $b_0 \in \mathbb{N}$, *such that, for any* $b > b_0$, *and any collection* $\underline{x} = (x_1, ..., x_b)$ *of distinct* k*-rational points on* C, *there is an admissible stability parameter* $\underline{a}^b \in \prod_{i=1}^b X^\star(B)^\vee_{\mathbb{Q},+}$ *of coprime type with the following property: for every principal* G*-bundle* $\mathscr{P}$ *with degree of instability* $\leq h$, *there exists a flagging* $\underline{s}$ *with* $s_i\colon \{x_i\} \to \mathscr{P}_{|\{x_i\}}/B$, $i = 1, ..., b$, *such that* $(\mathscr{P}, \underline{s})$ *is an* $\underline{a}^b$*-stable flagged principal* G*-bundle of type* $(\underline{x}^b, (B, ..., B))$.

Proof. Part v) of Lemma 4.2.1 shows that we may replace any stability parameter by one of coprime type, while enlarging the set of stable bundles. So we do not have to worry about the coprimality condition on $\underline{a}$.
Let $\mathrm{Bun}_G^{\vartheta;\leq h}$ be the stack of principal G-bundles of instability degree $\leq h$. This is an open substack of finite type of Bun_G [4]. Choose $a \in X^\star(B)^\vee_{\mathbb{Q},+}$, such that for all parabolic subgroups $Q \subset G$ one has either $\langle \det_Q, a \rangle > 0$ or $\langle \det_Q, a \rangle < -2h$. Such a choice is possible by Lemma 4.2.1, ii): we can find $a' \in X^\star(B)_{\mathbb{Q}}$, such that the finitely many values $\langle \det_Q, a' \rangle$ are all non-zero. Multiplying a' with a sufficiently large constant, we find a. Set

$$D := \max\{ \langle \det_Q, a \rangle \,|\, Q \subset G \text{ a parabolic subgroup} \}.$$

Note that this is a positive number.
Next, choose a sequence $(x_n)_{n\geq 1}$ of distinct points in $C(k)$, set $\underline{x}^b := (x_1, ..., x_b)$, and consider, for $b \in \mathbb{N}$, the stability parameter $\underline{a}^b := (a/b, \dots, a/b)$. It will be admissible for $b \gg 0$.

Observation. *Let* $\mathscr{P}$ *be a principal* G*-bundle,* $Q \subset G$ *a parabolic subgroup, and* $\mathscr{P}_Q$ *a reduction of* $\mathscr{P}$ *to* Q, *such that* $\deg(\mathscr{P}_Q) < -D$. *Then, for any*

b and any choice of sections $s_i\colon \{x_i\} \to \mathscr{P}_{|\{x_i\}}/B$, $i = 1, ..., b$, we have $\underline{a}^b$-$\deg(\mathscr{P}_Q) < 0$.

We want to estimate the dimension of the space of $\underline{a}^b$-unstable flagged principal G-bundles $(\mathscr{P}, \underline{s})$ of type $(\underline{x}^b, (B, ..., B))$ with $\mathscr{P} \in \mathrm{Bun}_G^{\vartheta, \leq h}$. First of all, the stack

$$\mathrm{Reductions} := \left\langle (\mathscr{P}, \mathscr{P}_Q) \;\middle|\; \begin{array}{l} \mathscr{P} \in \mathrm{Bun}_G^{\vartheta,\leq h}, \\ \mathscr{P}_Q \text{ a reduction of } \mathscr{P} \text{ to the parabolic} \\ \text{subgroup } Q \text{ with } \deg(\mathscr{P}_Q) \geq -D \end{array} \right\rangle$$

is an algebraic stack of finite type: reductions of a principal G-bundle $\mathscr{P}$ to Q are given by sections of $\mathscr{P}/Q$, and $\mathscr{P}/Q$ is projective over the base. Thus, by Grothendieck's construction of the quot schemes, these sections are parametrized by a countable union of quasi-projective schemes. We may apply this to the universal bundle over $\mathrm{Bun}_G^{\vartheta,\leq h} \times C$, because locally we may use the quot schemes for any bounded family over a scheme and the resulting schemes glue, because the functor is defined over the stack. The substack of reductions of fixed degree is of finite type, because the reduction is defined by the induced vector subbundle of the adjoint bundle of rank $\dim(Q)$ and the same degree as the reduction. In any bounded family of vector bundles, the vector subbundles of given rank and degree form also a bounded family. Finally, recall that we look only at degrees between $-D$ and h.
Therefore, the fiber product

$$\mathrm{Test} := \mathrm{Reductions} \times_{\mathrm{Bun}_G^{\vartheta,\leq h}} \mathrm{Bun}_{G,\underline{x}^b}^{\vartheta,\leq h}$$

parameterizing flagged principal G-bundles of type $(\underline{x}^b, (B, ..., B))$ together with a reduction of bounded degree to a parabolic subgroup is for any $b \in \mathbb{N}$ of finite type. Consider the closed substack Bad $\subset$ Test given by $(\mathscr{P}, \underline{s}, \mathscr{P}_Q)$ with $\underline{a}^b$-$\deg(\mathscr{P}_Q) \geq 0$. We can estimate the dimension of the fibers of Bad $\to$ Reductions as follows: fix $\mathscr{P} \in \mathrm{Bun}_G^{\vartheta,\leq h}$, a parabolic subgroup $Q \subset G$, and a reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to Q. Given b, the variety of flaggings of $\mathscr{P}$ is $\times_{i=1}^b \mathscr{P}_{|\{x_i\}}/B \cong (G/B)^{\times b}$. Now, for every i, the subset

$$\left\{ s_i \in \mathscr{P}_{|\{x_i\}}/B \,|\, \langle \det_Q, a_{s_i} \rangle < 0 \right\} \subset \mathscr{P}_{x_i}/B$$

is non-empty and open. Denote its complement by Z_i. Now, if $\#\{i | s_i \notin Z_i\} > b \cdot (h + D)/(2h + D)$, then $(\mathscr{P}, \underline{s})$ is $\underline{a}^b$-stable: indeed, we compute

$$\begin{aligned} \underline{a}^b\text{-}\deg(\mathscr{P}_Q) &= \deg(\mathscr{P}_Q) + \sum_{i=1}^b \langle \det_Q, a_{s_i} \rangle \\ &< h - b \cdot \frac{h+D}{2h+D} \cdot \frac{2h}{b} + b \cdot \left(1 - \frac{h+D}{2h+D}\right) \cdot \frac{D}{b} = 0. \end{aligned}$$

Thus,

$$\dim(\mathrm{Bad}) \leq \dim(\mathrm{Reductions}) + b \cdot \dim(G/B) - b \cdot \frac{h}{2h+D}.$$

Thus, for $b \gg 0$, we see that $\dim(\mathrm{Bad}) < b \cdot \dim(G/B)$ and therefore the image of Bad in $\mathrm{Bun}_{G,\underline{x}^b}^{\vartheta,\leq h}$ cannot contain any fiber of $\mathrm{Bun}_{G,\underline{x}^b}^{\vartheta,\leq h} \to \mathrm{Bun}_G^{\vartheta,\leq h}$. □

Remark 4.2.3. The proof also shows that we may make the codimension of the locus of $\underline{a}^b$-unstable flagged principal G-bundles as large as we wish.

4.3 The Canonical Reduction for Flagged Principal Bundles

Motivated by work of Harder [20], Stuhler explained in [41] how to define a notion of stability for Arakelov group schemes over curves and how to use Behrend's technique of complementary polyhedra to prove the existence of a canonical reduction to a parabolic subgroup in this situation. We only had to translate this to our special case of flagged principal G-bundles. According to Behrend, it suffices to show that the parabolic degree defined above defines a complementary polyhedron, a concept which we will recall below. All the results of this section are due to Behrend [6] (with some simplifications given by Harder and Stuhler in the above references). We only have to verify that his theory applies to our situation. Since in our case of flagged principal bundles the arguments simplify a bit, we will try to give a self-contained account.
Let $(\mathscr{P}, \underline{s})$ be a flagged principal G-bundle on C and fix a stability parameter $\underline{a}$. Let $P \subset G$ be a parabolic subgroup. A reduction $\mathscr{P}_P$ of $\mathscr{P}$ to P is called *canonical*, if

(1) $\underline{a}$-$\deg(\mathscr{P}_P) = \mathrm{ideg}_{\underline{a}}(\mathscr{P}, \underline{s})$.

(2) P is a maximal element in the set of parabolic subgroups for which there is a reduction $\mathscr{P}_P$ of degree $\mathrm{ideg}_{\underline{a}}(\mathscr{P}, \underline{s})$.

Remark 4.3.1. Let $\mathscr{P}_P$ be a canonical reduction of $\mathscr{P}$ and denote by $R_u(P)$ the unipotent radical of P. Note that by Remark 4.1.2, iii), the induced principal $(P/R_u(P))$-bundle $\mathscr{P}_P/R_u(P)$ inherits a flagging $\underline{s}'$: indeed, we may choose a representative for a_{s_i} which lies in a maximal torus of $\mathrm{Aut}(\mathscr{P})_{|\{x_i\}}$ which is contained in the intersection of the parabolic subgroup given by the flagging at x_i with the parabolic subgroup given by the canonical reduction and define the parabolic subgroup of $\mathrm{Aut}(\mathscr{P}_P/R_u(P))_{|\{x_i\}}$ associated with a_{s_i} as the flagging s'_i of $\mathscr{P}_P/R_u(P)$ at x_i, $i = 1, ..., b$. Using this, we find that $\mathscr{P}_P$ has the following properties:

(1′) $(\mathscr{P}_P/R_u(P), \underline{s}')$ is an $\underline{a}$-semistable flagged principal bundle.
This holds, because the preimage of a reduction of positive degree of $\mathscr{P}_P/R_u(P)$ would define a parabolic reduction of larger degree in $\mathscr{P}$.

(2′) For all parabolic subgroups P' containing P, one has the inequality $\underline{\underline{a}\text{-}\deg}(\mathscr{P}_P)(\det_P \otimes \det_{P'}^{-1}) > 0$. In fact, by the definition of a canonical reduction, we know that $\underline{\underline{a}\text{-}\deg}(\mathscr{P}_P)(\det_{P'}) = \underline{a}\text{-}\deg(\mathscr{P}_{P'}) < \underline{a}\text{-}\deg(\mathscr{P}_P) = \underline{\underline{a}\text{-}\deg}(\mathscr{P}_P)(\det_P)$.

We can now state the analog of Behrend's theorem for flagged principal bundles:

Theorem 4.3.2. *Let* $(\mathscr{P}, \underline{s})$ *be a flagged principal* G*-bundle and* $\underline{a}$ *an admissible stability parameter. Then, there is a unique reduction of* $\mathscr{P}$ *to a parabolic subgroup* $P \subset G$*, satisfying the above conditions* $(1')$ *and* $(2')$*. Moreover, this is a canonical reduction of* $(\mathscr{P}, \underline{s})$*.*

Let us rewrite Behrend's proof in our situation. Since canonical reductions of $\mathscr{P}$ exist, only the uniqueness has to be proved. Thus, fix two parabolic subgroups P and Q of G and let $\mathscr{P}_P$ and $\mathscr{P}_Q$ be reductions of $\mathscr{P}$ to P and Q, respectively. Since any two parabolic subgroups share a maximal torus, we may assume that, locally at the generic point $\eta \in C$, there is a reduction $\mathscr{P}_{T,\eta}$ of $\mathscr{P}$ to a torus $T \subset P \cap Q$, such that $\mathscr{P}_{P,\eta} = \mathscr{P}_{T,\eta} \times^T P$ and $\mathscr{P}_{Q,\eta} = \mathscr{P}_{T,\eta} \times^T Q$ as subbundles of $\mathscr{P}$.
Note further that any reduction of the generic fiber of $\mathscr{P}$ to a parabolic subgroup canonically extends to a reduction of $\mathscr{P}$, so that $\mathscr{P}_P$ and $\mathscr{P}_Q$ are determined by $\mathscr{P}_{P,\eta}$ and $\mathscr{P}_{Q,\eta}$, respectively. We therefore fix a reduction $\mathscr{P}_{T,\eta}$. For any parabolic subgroup $T \subset P \subset G$, this defines a reduction $\mathscr{P}_P$ of $\mathscr{P}$, and we only need to study how the degree of $\mathscr{P}_P$ varies with P. Finally, given a Borel subgroup $T \subset B \subset P$, the parabolic degree $\underline{a}\text{-}\underline{\deg}(\mathscr{P}_B)$ determines $\underline{\underline{a}\text{-}\deg}(\mathscr{P}_P)$. Thus, like Behrend, we consider these degrees as a map:

$$\begin{aligned} d\colon \big\{\, T \subset B \subset G \,|\, \text{Borel subgroup}\,\big\} &\longrightarrow X^\star(T)^\vee \\ B &\longmapsto \underline{a}\text{-}\underline{\deg}(\mathscr{P}_B). \end{aligned}$$

This map is a "complementary polyhedron", i.e., it satisfies:

(P1) If B and B' are two Borel subgroups contained in the parabolic subgroup $P \subset G$, then $d(B)_{|X^\star(P)} = d(B')_{|X^\star(P)}$.

(P2) Let B and B' be two Borel subgroups, such that the simple roots of B are $I_B = \{\alpha, \alpha_1, \ldots \alpha_{r-1}\}$ and $\{-\alpha\} = -I_B \cap \varDelta_{B'}$. Then, $d(B)(\alpha) + d(B')(-\alpha) \leq 0$.

(P1) is clear, since both sides only depend on the reduction of $\mathscr{P}$ to P.
To see (P2), let L be a Levi subgroup of $P_\alpha := BB'$, and set $L' := P_\alpha/R_u(P_\alpha)Z(L) \cong L/Z(L)$. Then, $\mathscr{L} := \mathscr{P}_\alpha/R_u(P_\alpha)Z(L)$ is the principal L'-bundle obtained from $\mathscr{P}_{P_\alpha}$ by extension of the structure group via $P_\alpha \to L'$, and we may compute $d(B)(\alpha)$ and $d(B')(\alpha)$ from $\mathscr{L}$ and the induced reductions. Thus, by replacing G by L', we may assume that G is semisimple of rank one and that B and B' define reductions $\mathscr{L}_B$ and $\mathscr{L}_{B'}$ of $\mathscr{L}$ which are opposite at the generic point. Denote by $\mathfrak{g}$, $\mathfrak{b}$, and $\mathfrak{b}'$ the Lie algebras of G, B, and B', respectively, and by $\mathfrak{u}_\alpha$ the root space of α.
Since the reductions are opposite in the generic fiber, the composition

$$\mathscr{L}_B \times^B \mathfrak{u}_\alpha \subset \mathscr{L}_B \times^B \mathfrak{g} = \mathscr{L}_{B'} \times^{B'} \mathfrak{g} \to \mathscr{L}_{B'} \times^B \mathfrak{g}/\mathfrak{b}'$$

is non-zero, i.e., there is an injective map of line bundles $\mathscr{L}_B(\alpha) \to \mathscr{L}_{B'}(\alpha)$.
If this map is an isomorphism at x_i, then $\mathscr{L}_B$ and $\mathscr{L}_{B'}$ are opposite in this fiber. In this case, if s_i defines a reduction to either $\mathscr{L}_{B,x_i}$ or $\mathscr{L}_{B',x_i}$, then

$\langle\alpha, a_{s_i}\rangle_{\mathscr{L}_B} + \langle-\alpha, a_{s_i}\rangle_{\mathscr{L}_{B'}} = 0$, and, if the reduction is different from $\mathscr{L}_{B,x_i}$ and $\mathscr{L}_{B',x_i}$, then $\langle\alpha, a_{s_i}\rangle_{\mathscr{L}_B} = \langle-\alpha, a_{s_i}\rangle_{\mathscr{L}_{B'}} \le 0$. (Note that by our reduction to the case of semisimple rank one, there are only two possible values for the product $\langle.,.\rangle$, by Lemma 4.1.3). If the map is not an isomorphism at x_i, then $\deg(\mathscr{L}_B(\alpha)) \le \deg(\mathscr{L}_{B'}(\alpha)) - 1$. Thus, our claim follows again, because we have chosen $\underline{a}$ to be admissible, i.e., $2|\langle\alpha, a_i\rangle| < 1$. Altogether, we have established (P2). In the case $G = \mathrm{SL}_3$, the above properties imply that the points $d(B)$ are the corners of a hexagon whose sides are parallel to the coroots. This might motivate the following observation of Behrend. (For any $M \subset X^\star(T)^\vee$, denote by $\mathrm{conv}(M)$ the convex hull of M (in $X^\star(T)^\vee_{\mathbb{R}}$).)

Lemma 4.3.3 ([6], Lemma 2.5). *With the above notation, we have*

$$\mathrm{conv}\big(\{\, d(B) \,|\, T \subset B \,\}\big) = \bigcap_{\substack{P \supset T \\ P \text{ max. par.}}} \Big\{\, x \in X^\star(T)^\vee \,|\, x(\det_P) \ge \underline{\underline{a}\text{-}\deg}(\mathscr{P}_P)(\det_P) \,\Big\}.$$

In particular, if $(\mathscr{P}, \underline{s})$ is semistable, then this convex set contains 0.

Note that, for a maximal parabolic subgroup P, the space $X^\star(P)_{\mathbb{Q}}$ is one dimensional, so that in the above we might replace $\det_P$ by any dominant character $\lambda \in X^\star(P)_{\mathbb{Q}}$.

Proof. Again, given a parabolic subgroup $P \supset T$, denote by Δ_P the set of roots of P and, given a Borel subgroup $B \supset T$, by I_B the set of positive simple roots.

To prove the inclusion "$\subset$", we fix P and show that $d(B)(\det_P) \ge d(P)(\det_P)$. If $B \subset P$, then this holds by definition. Otherwise, let $-\alpha_0 \in I_B \setminus \Delta_P$ be a simple root of B which is not a root of P, so that $\alpha_0 \in \Delta_P$. Let B' be the Borel subgroup that differs from B by α_0, and let P_{α_0} be the parabolic subgroup generated by BB'. If we show that $\det_P = \lambda_{\alpha_0} + m\alpha_0$, with $\lambda_{\alpha_0} \in X^\star(P_{\alpha_0})_{\mathbb{Q}}$ and $m \ge 0$, then, by the properties (P1) and (P2) of d, we see that

$$\begin{aligned} d(B)(\det_P) &= d(B)(\lambda_{\alpha_0}) + md(B)(\alpha_0) \\ &\ge d(B')(\lambda_{\alpha_0}) + md(B')(\alpha_0) = d(B')(\det_P). \end{aligned}$$

Iterating this procedure, we finally arrive at the case $B \subset P$.

Let $(.,.)$ be a W-invariant scalar product on $X^\star(T)_{\mathbb{Q}}$. Define $\alpha_0^\vee$, such that the reflection s_{α_0} is given as $\lambda \mapsto \lambda - (\lambda, \alpha_0^\vee)\alpha_0$. Then, we need to show that $(\det_P, \alpha_0^\vee) \ge 0$. Recall that $\det_P = \sum_{\alpha \in \Delta_P} \alpha$. For a root $\alpha \in \Delta_P$ with $(\alpha, \alpha_0^\vee) < 0$, we know that $s_{\alpha_0}(\alpha) \in \Delta_P$, because $\alpha_0, \alpha \in \Delta_P$, and $(s_{\alpha_0}(\alpha), \alpha_0^\vee) = -(\alpha, \alpha_0^\vee)$. Thus, our assertion is trivial.

To prove the other inclusion, Behrend proceeds by induction on the rank of G. The claim holds, if $X^\star(T)$ is one dimensional. Let $P \supset T$ be a maximal parabolic subgroup with Levi subgroup L. Then, the polyhedron for the associated Levi bundle is given by

$$\begin{aligned} &\mathrm{conv}\big(\{\, d(B) \,|\, T \subset B \subset P \,\}\big) \\ &\quad \subset \big\{\, \varphi \in X^\star(T)^\vee_{\mathbb{Q}} \,|\, \varphi(\det_P) = \underline{a}\text{-}\deg(\mathscr{P}_P)(\det_P) \big\} \cong X^\star(T/Z(L))^\vee_{\mathbb{Q}}. \end{aligned}$$

Now, in the first step of the proof, we have seen that, for any Borel subgroup $B \supset T$, either $d(B)(\det_P) > \underline{a}\text{-deg}(\mathscr{P}_P))$ or $d(B) = d(B')$ for some Borel subgroup $B' \subset P$. Thus,

$$\operatorname{conv}\bigl(\{\, d(B) \,|\, T \subset B \,\}\bigr) \cap \{\, \varphi \,|\, \varphi(\det_P) = \underline{a}\text{-deg}(\mathscr{P}_P) \,\} \\ = \operatorname{conv}\bigl(\{\, d(B) \,|\, T \subset B \subset P\}\bigr).$$

This shows that the $d(B)$ also span the intersection of the halfspaces. □

Again, fix a scalar product $(.,.)$ on $X^\star(T)^\vee_{\mathbb{Q}}$ which is invariant under the action of the Weyl group of G. Then, Behrend's theorem follows immediately from:

Proposition 4.3.4 ([6], Proposition 3.13). *Let $\mathscr{P}_Q$ be a reduction of $\mathscr{P}$ satisfying* (1′) *and* (2′)*, and let $\mathscr{P}_{T,\eta}$ be a reduction of $\mathscr{P}_Q$ to T at the generic point of C. Then, $\mathscr{P}_Q$ is also defined as the reduction to the parabolic subgroup associated with the rational one-parameter subgroup of least distance to the origin in* $\operatorname{conv}(\{\, d(B) \,|\, T \subset B \,\})$.

Proof. Again, let $Q \subset G$ be the parabolic subgroup corresponding to the reduction $\mathscr{P}_Q$, and let L be a Levi subgroup of Q. The intersection

$$\bigcap_{\substack{P \supset Q \\ P \text{ max. parabolic}}} \{\, x \in X^\star(T)^\vee_{\mathbb{Q}} \,|\, x(\det_P) = \underline{a}\text{-deg}(\mathscr{P}_P) \,\} \cap X^\star(Z(L))^\vee_{\mathbb{Q}}$$

contains only one point, call it y_Q. Indeed, $X^\star(Q)_{\mathbb{Q}} \cong X^\star(Z(L))_{\mathbb{Q}}$ and, if $P_i \supset Q$, $i = 1, \ldots, m$, are the maximal parabolic subgroups containing Q, then $(\det_{P_i})_{i=1,\ldots,m}$ is a basis for $X^\star(Q)_{\mathbb{Q}}$.
Claim 1: Under the identification $X^\star(T)^\vee \cong X_\star(T)$, the parabolic subgroup defined by $y_Q \in X_\star(T)$ is Q.
First, $y_Q \in X^\star(Z(L))^\vee$ implies that $y_Q \in X_\star(Z(L))_{\mathbb{Q}}$. Furthermore, since the characters $\det_{P_i}$, $i = 1, ..., m$, form a basis of $X^\star(Q)_{\mathbb{Q}}$, we have $y_Q(\det_P) = \underline{a}\text{-deg}(\mathscr{P}_Q)(\det_P)$, for all maximal parabolic subgroups $P \supset Q$. Therefore, property (2′) of $\mathscr{P}_Q$ implies that the parabolic subgroup associated with y_Q is Q (compare the comments before Remark 4.1.2).
Claim 2: $y_Q \in \operatorname{conv}(\{\, d(B) \,|\, T \subset B \subset Q \,\}) \subset \operatorname{conv}(\{\, d(B) \,|\, T \subset B \,\})$.
We have the exact sequence

$$X^\star(Z(L))^\vee_{\mathbb{Q}} \longrightarrow X^\star(T)^\vee_{\mathbb{Q}} \xrightarrow{\pi} X^\star(T/Z(L))^\vee,$$

and $\pi(\operatorname{conv}\{\, d(B) \,|\, T \subset B \subset Q \,\})$ is the polyhedron of the Levi bundle $\mathscr{P}_Q/R_u(Q)$, which is semistable by assumption. In particular, $0 \in \pi(\operatorname{conv}\{\, d(B) \,|\, T \subset B \subset Q \,\})$ (Lemma 4.3.3). Thus, $\operatorname{conv}(\{\, d(B) \,|\, T \subset B \subset Q \,\}) \cap X^\star(Z(L))^\vee \neq \varnothing$, and y_Q is the only point that can be contained in this intersection.
Claim 3: Under the identification $X^\star(T)^\vee_{\mathbb{R}} \cong X^\star(T)_{\mathbb{R}}$ given by the W-invariant scalar product $(.,.)$, we have $y_Q = \sum_{i=1}^m n_i \det_{P_i}$ with $n_i > 0$, $i = 1, ..., m$.

First, $X^\star(Q)_\mathbb{R} \cong X^\star(Z(L))_\mathbb{R}$ is the intersection of the subspaces invariant under the reflections s_{α_i}, for $\alpha_i \in I_B \setminus I_Q$, i.e., $X^\star(Q)_\mathbb{R} = (\bigoplus_{\alpha_i \in I_B \setminus I_Q} \mathbb{R}\alpha_i)^\perp$. In particular, $X^\star(Z(L))_\mathbb{R}^\vee$ is the subspace that is invariant under the Weyl group W_L of L.
Let $B \subset Q$ be a Borel subgroup, α_i a simple root of B for which $-\alpha_i$ is not a root of Q, and $P_i^{\min}$ the parabolic subgroup obtained from Q by adding the root α_i, $i = 1, ..., m$. Define $\widetilde{\alpha}_i := \det_Q \otimes \det^{-1}_{P_i^{\min}} \in X^\star(Q)$, $i = 1, ..., m$. Then, $\widetilde{\alpha}_i = l\alpha_i + \sum_{\beta \in I_B \setminus I_Q} l_\beta \beta \in X^\star(Q)$ with $l > 0, l_\beta \geq 0$, $i = 1, ..., m$. Therefore, $\widetilde{\alpha}_i$ is the l-fold multiple of the orthogonal projection of α_i to $X^\star(Q)$, $i = 1, ..., m$. Moreover, $\det_{P_i}$ is invariant under the reflection s_α, for $\alpha \in I_B \setminus \{\alpha_i\}$, $i = 1, ..., m$. Since $\widetilde{\alpha}_i$ and $\det_{P_i}$ are both positive linear combinations of the simple roots, we find that $(\det_{P_j}, \widetilde{\alpha}_k) = c_j \delta_{jk}$ with $c_j > 0$, $j, k = 1, ..., m$. Now, $y_{Q|X^\star(Q)} = \underline{a}\text{-deg}(\mathscr{P}_Q)$ and $\deg(\mathscr{P}_Q)(\widetilde{\alpha}_i) > 0$, $i = 1, ..., m$, because $\mathscr{P}_Q$ satisfies (2′). We infer $y_Q = \sum_{i=1}^m n_i \det_{P_i}$ with $n_i > 0$, for $i = 1, ..., m$.
Claim 4: y_Q is the point of least distance to 0 in $\operatorname{conv}(d(B))$.
We have seen in Lemma 4.3.3 that

$$\operatorname{conv}\big(\{\, d(B) \,|\, T \subset B \,\}\big) = \bigcap_{\substack{P \supset T \\ P \text{ max. parabolic}}} \big\{\, x \in X^\star(T)^\vee \,|\, x(\det_P) \geq \underline{a}\text{-deg}(\mathscr{P}_P) \,\big\}.$$

Thus, for any $x \in \operatorname{conv}(\{\, d(B) \,|\, T \subset B \,\})$ and any $i \in \{\, 1, ..., m \,\}$, we have $x(\det_{P_i}) > \underline{a}\text{-deg}(\mathscr{P}_Q)(\det_{P_i}) = y_Q(\det_{P_i})$. Since $y_Q = \sum_{i=1}^m n_i \det_{P_i}$ with $n_i \geq 0$, $i = 1, ..., m$, we see that

$$(x - y_Q, y_Q) = \sum_{i=1}^m n_i \big(x(\det_{P_i}) - y_Q(\det_{P_i})\big) \geq 0,$$

so that $\|x\| \geq \|y_Q\|$. □

4.4 Semistable Reduction for Flagged Principal Bundles

Following our strategy from [22],[23], we want to prove a semistable reduction theorem for flagged principal bundles.

Theorem 4.4.1. *Let C be a smooth projective curve over the discrete valuation ring R with residue field k. Let $\{\, x_i \colon \operatorname{Spec}(R) \to C \,|\, i = 1, \ldots, b \,\}$ be a finite set of disjoint sections, G a semisimple Chevalley group scheme over R, $\underline{P}$ a tuple of parabolic subgroups of G, and $\underline{a}$ an admissible stability parameter.*
Then, for any $\underline{a}$-semistable flagged principal G-bundle $(\mathscr{P}_K, \underline{s}_K)$ over C_K, there is a finite extension $R' \supset R$, such that $(\mathscr{P}_K, \underline{s}_K)$ extends to an $\underline{a}$-semistable flagged principal G-bundle over $C_{R'}$.

Proof. In order to ease notation, we will assume that $P_i = B$, $i = 1, ..., b$, for a fixed Borel subgroup B of G. For our main application, this case is sufficient. The other cases are proved in the same way. Write $S = \{\, x_1, \ldots, x_b \,\}$, and consider S as a closed subscheme of C.

First Step: Find an arbitrary extension of $\mathscr{G}_K$ to $C_{R'}$.
We know ([22], First Step) that, after replacing R by a finite extension, we can always extend the principal G-bundle $\mathscr{P}_K$ to a principal bundle $\mathscr{P}_R$ over C_R. The reductions of $\mathscr{P}_{R|S}$ are parameterized by a scheme which is locally (over R) isomorphic to $G/B \times_R S$. Since this scheme is projective over R, the flaggings of $\mathscr{P}_{K|K\times_R S}$ extend uniquely to flaggings s_i of $\mathscr{P}_{R|S}$, $i = 1, ..., b$.
Second Step: Find a modification of $(\mathscr{P}_R, \underline{s})$.
Fix a local parameter $\pi \in R$. Assume that $(\mathscr{P}_k, \underline{s})$ is not semistable. Then, by Theorem 4.3.2, there is a canonical reduction of $\mathscr{P}_k$ to a parabolic subgroup $P \subset G$. Let $T \subset B \cap P$ be a maximal torus of G. The relative position of the reduction to P and to B at x_i is given by an element of $P\backslash G/B \cong W_P\backslash W$, $i = 1, ..., b$. Here, $W = N(T)/T$ is the Weyl group of G, and W_P is the Weyl group of the Levi quotient of P. For $i = 1, \dots, b$, we choose an element $w_i \in N(T)$ which defines the relative position at x_i.
We want to describe $(\mathscr{P}_R, \underline{s})$ by a glueing cocycle. Recall that any $g \in \prod_S G(\!(t)\!)(R)$ defines a principal G-bundle $\mathscr{P}_g$ on C together with a trivialization of the restrictions $\mathscr{P}_{g|C\setminus S}$ and $\mathscr{P}_{g|\widehat{\mathscr{O}}_{C,S}}$. In particular, the latter trivialization also defines flaggings at S.
As in [22], we choose a maximal parabolic subgroup $Q \supset P$. Then, there is a finite, disjoint set of sections U, such that we can find a cocycle $g \in \prod_S G(\!(t)\!)(R) \times \prod_U G(\!(t)\!)(R)$ and $g_0 \in \prod_S G(R)$, satisfying the following:

(1) gg_0 defines $(\mathscr{P}_R, \underline{s})$

(2) $g \mod \pi \in \prod_{S\cup U} P(\!(t)\!)(k)$ defines the canonical reduction of $\mathscr{P}_k$ to P.

(3) $(g_0)_{x_i\in S} \mod \pi = (w_i)_{x_i\in S} \in N(T)(k)$.

(4) Either g satisfies the conditions of [22], Proposition 7, or $g \in \prod_{S\cup U} P(\!(t)\!)(R)$.

(5) If $g \in \prod_{S\cup U} P(\!(t)\!)(R)$, then the maximal N, such that $(g_0)_{x_i\in S} \equiv (w_i)_{x_i\in S} \mod \pi^N$ is finite. Furthermore, $(g_0)_{x_i\in S} \mod \pi^{N+1} \notin \prod_{x_i\in S} Pw_iB$.

For the above cocycle gg_0, choose $z = \pi^{\ell/N}$ with ℓ maximal, such that the cocycle $zgg_0(w^{-1}z^{-1}w) = zgz^{-1}zg_0(w^{-1}z^{-1}w)$ is an $R[\pi^{1/N}]$-valued cocycle. This defines a flagged principal G-bundle $(\mathscr{P}', \underline{s}')$ which is another extension of $(\mathscr{P}_K, \underline{s}_K)$.
Third Step: Show that $(\mathscr{P}'_k, \underline{s}')$ is less unstable.
The Harder–Narasimhan strata (HN-strata) that we shall consider in the following are understood as Harder–Narasimhan strata in the stack $\mathrm{Bun}_{G,\underline{x},\underline{P},\underline{a}}$ of flagged principal G-bundles of type $(\underline{x}, \underline{P})$ with respect to the stability parameter $\underline{a}$.

Lemma 4.4.2. *Let $(\mathscr{P}_\eta, \underline{s})$ be a flagged principal G-bundle which specializes to the flagged principal G-bundle $(\mathscr{P}_0, \underline{s})$, i.e., assume that there is a family of* *flagged principal G-bundles parameterized by the complete discrete valuation ring R with special fiber $(\mathscr{P}_0, \underline{s})$ and generic fiber $(\mathscr{P}_\eta, \underline{s})$. Assume further that $(\mathscr{P}_\eta, \underline{s})$ has a canonical reduction defined over the generic point of R. Then, $\mathrm{ideg}_{\underline{a}}(\mathscr{P}_\eta, \underline{s}) \leq \mathrm{ideg}_{\underline{a}}(\mathscr{P}_0, \underline{s})$. If the flagged principal G-bundles $(\mathscr{P}_\eta, \underline{s})$ and $(\mathscr{P}_0, \underline{s})$ do not lie in the same HN-stratum, then $\mathrm{ideg}_{\underline{a}}(\mathscr{P}_\eta, \underline{s}) < \mathrm{ideg}_{\underline{a}}(\mathscr{P}_0, \underline{s})$.*

Proof. Let $\mathscr{P}_{P,\eta}$ denote the canonical reduction of $(\mathscr{P}_\eta, \underline{s})$. This induces a reduction $\mathscr{P}_{0,P}$ of the generic fiber by first extending the reduction to an open subset of the special fiber and then extending this to a reduction over the special fiber. Let us compare the contributions of the flaggings at the point x_i, $i = 1, ..., b$. First assume that the reduction $\mathscr{P}_{P,\eta}$ extends to the special fiber, locally at the point x_i. In this case, this extension coincides with $\mathscr{P}_{0,P}$ and we can apply the semicontinuity argument of Example 4.1.4 to see that the contribution of $\langle \det_P, a_i \rangle$ can at most increase in the special fiber.
In the other case, the reduction $\mathscr{P}_{P,\eta|\{x_i\}}$ can also be extended to a reduction of $\mathscr{P}_{x_i}$. We denote the corresponding reduction by $\mathscr{P}_{P,x_i}$. To this reduction, we can apply the same argument as before to see that the corresponding value of $\langle \det_P, a_i \rangle$ can at most increase in the special fiber.
Finally, let $\mathscr{P}^{\max}_{\mathfrak{p}}$ be the maximal subsheaf of $\mathscr{P} \times^G \mathrm{Lie}(G)$ that extends $\mathscr{P}_{\eta,P} \times^P \mathrm{Lie}(P)$. Then, in the special fiber over x_i, we have

$$\mathscr{P}^{\max}_{\mathfrak{p}|\{\,x_i,0\,\}} \subset \mathscr{P}_{x_i,P} \times^P \mathrm{Lie}(P) \cap \mathscr{P}_{0,P} \times^P \mathrm{Lie}(P)_{|\{\,x_i,0\,\}}, \quad i = 1, ..., b.$$

Since $\underline{a}$ is admissible, this implies

$$\begin{aligned}\mathrm{ideg}(\mathscr{P}_\eta, \underline{s}) &\leq \underline{a}\text{-}\mathrm{deg}(\mathscr{P}_{0,P}, \underline{s})(\det(P)) - \\ &\quad - \deg\big(\mathrm{coker}(\mathscr{P}^{\max}_{\mathfrak{p},0} \to \mathscr{P}_{0,P} \times^P \mathrm{Lie}(P)\big) \cdot \\ &\qquad \cdot \big(1 - 2 \cdot \max\{\, |\langle \alpha, a_i \rangle| \,|\, \alpha \text{ a root of } G, i = 1, \dots, b \,\}\big) \\ &\leq \mathrm{ideg}(\mathscr{P}_0, \underline{s}).\end{aligned}$$

Therefore, we see that either $\mathrm{ideg}(\mathscr{P}_\eta) < \mathrm{ideg}(\mathscr{P}_0)$, or the canonical reduction $\mathscr{P}_P$ defines a reduction of $\mathscr{P}_0$ of the same parabolic degree, which must then be the canonical reduction by Theorem 4.3.2. □

Lemma 4.4.3. *Let $\mathscr{P}$ be a principal G-bundle and $(\mathscr{P}, \underline{s})$ and $(\mathscr{P}, \underline{s}')$ two flaggings of $\mathscr{P}$ of the same type. Let $\mathscr{P}_P$ be the canonical reduction of $(\mathscr{P}, \underline{s})$, and denote by w_i and $w'_i \in P\backslash G/B$ the elements defined by the relative position of the two reductions of $\mathscr{P}_{|\{x_i\}}$ to P and B given by s_i and s'_i, respectively, $i = 1, ..., b$. Assume that w'_i specializes to w_i, $i = 1, ..., b$. Then, $(\mathscr{P}, \underline{s}')$ is less unstable than $(\mathscr{P}, \underline{s})$.*

Proof. Since $\underline{s}'$ specializes to $\underline{s}$, we can apply Lemma 4.4.2 to see that $\mathrm{ideg}(\mathscr{P}, \underline{s}) \geq \mathrm{ideg}(\mathscr{P}, \underline{s}')$. Assume that both flagged principal G-bundles lie in the same HN-stratum. Then, the canonical reduction of $(\mathscr{P}, \underline{s}')$ defines another reduction $\mathscr{P}'_P$ of $\mathscr{P}$ to P. Now, we may use Example 4.1.4 to see that the parabolic degree of $(\mathscr{P}'_P, \underline{s})$ is bigger than the parabolic degree of $(\mathscr{P}_P, \underline{s}')$, because $w \neq w'$. □

Finally, as in [22], third step, choose a Levi subgroup L of Q, set $\mathscr{P}_Q := \mathscr{P}_P \times^P Q$, and consider the family $\mathscr{Q}_\lambda$ of principal Q-bundles over $C_k \times \mathbb{A}^1$ that is isomorphic to $\mathscr{P}_Q \times \mathbb{G}_m$ over $C \times \mathbb{G}_m$ and such that the fiber over 0 is $\mathscr{P}_Q/R_u(Q) \times^L Q$. Set $\mathscr{P}_\lambda := \mathscr{Q}_\lambda \times^Q G$. Note that the flagging of $\mathscr{P}_k$ induces a flagging for the whole family $(\mathscr{P}_\lambda, \underline{s}_\lambda)$; denote by $(\mathscr{P}_0, \underline{s}_0)$ the fiber over 0 of this family.

Lemma 4.4.4. *The flagged principal G-bundles $(\mathscr{P}_0, \underline{s}_0)$ and $(\mathscr{P}_k, \underline{s})$ lie in the same HN-stratum of* $\mathrm{Bun}_{G,\underline{x},\underline{P},\underline{a}}$.

Proof. The principal P-bundle $\mathscr{P}_P$ also defines a reduction $\mathscr{P}_{0,P}$ of $\mathscr{P}_0$ to P. For this reduction, $\underline{\underline{a}\text{-deg}}(\mathscr{P}_{0,P}) = \underline{\underline{a}\text{-deg}}(\mathscr{P}_P)$, because all terms in the definition of the degree depend only on the quotient of $\mathscr{P}_P/R_u(P)$. By Behrend's characterization of the canonical reduction, this implies that $\mathscr{P}_{0,P}$ is the canonical reduction of $\mathscr{P}_0$. □

Corollary 4.4.5. *The flagged principal G-bundle $(\mathscr{P}'_k, \underline{s}')$ is less unstable than $(\mathscr{P}_k, \underline{s})$.*

Proof. As in the case of principal bundles, we only need to compare the HN-strata of $(\mathscr{P}'_k, \underline{s}')$ and $(\mathscr{P}_k, \underline{s})$. If $\mathscr{P}'$ and $\mathscr{P}$ are isomorphic as principal G-bundles (i.e., without flagging), then the cocycle used to define $\mathscr{P}'$ satisfies (5). Then, we know that the element g'_0 specializes to w, in which case Lemma 4.4.3 proves our claim.
Otherwise, we can argue as in the case of principal bundles [23] to see that the reduction of $\mathscr{P}_0$ to Q does not lift to $\mathscr{P}'$. So, again we know that $\mathscr{P}'$ is less unstable. □

As in the case of principal bundles without flaggings, we can now argue as follows: start with an arbitrary unstable extension $(\mathscr{P}, \underline{s})$ of the flagged principal bundle $(\mathscr{P}_K, \underline{s}_K)$. Either the special fiber of $(\mathscr{P}, \underline{s})$ is semistable, or we can find another extension $(\mathscr{P}', \underline{s}')$ which is less unstable. Since the instability degree of $(\mathscr{P}, \underline{s})$ is finite, this process will stop after finitely many iterations. □

5 Construction of the Moduli Spaces

We will now carry out the GIT construction of the moduli spaces of flagged principal G-bundles. The strategy is roughly the same as in the case of principal G-bundles ([36], [38], [15]), i.e., we first introduce flagged pseudo G-bundles whose moduli spaces can be constructed with the help of decorated flagged vector bundles and then explain how we obtain the moduli spaces of flagged principal G-bundles from there. At the end, we will give the full construction of the moduli space of decorated flagged vector bundles, following and generalizing [37].

5.1 Reduction to a Problem for Decorated Vector Bundles

Fix the type $(\underline{x}, \underline{P})$ of the flagging and the semistability parameter $\underline{a}$. We want to adapt the construction of moduli spaces for principal bundles given in [15] to flagged principal G-bundles. Thus, we will fix a faithful representation $\varrho\colon G \longrightarrow \mathrm{SL}(V) \subset \mathrm{GL}(V)$ on a finite dimensional k-vector space V. Given a principal G-bundle $\mathscr{P}$ over C, we write $\mathscr{P}(V)$ or $\mathscr{P}(\varrho)$ for the vector bundle with fiber V that is associated with G via the representation ϱ, $\mathscr{P}_{\mathrm{SL}(V)} := \mathscr{P} \times^G \mathrm{SL}(V)$ for the corresponding principal $\mathrm{SL}(V)$-bundle, and $\mathscr{P}_{\mathrm{GL}(V)} := \mathscr{P} \times^G \mathrm{GL}(V)$ for the associated principal $\mathrm{GL}(V)$-bundle.

ϱ-Flagged Principal G-Bundles. — Let $\underline{P} = (P_1, ..., P_b)$ be a tuple of parabolic subgroups of $\mathrm{GL}(V)$. As before, we fix a tuple $\underline{x} = (x_1, ..., x_b)$ of distinct k-rational points. Then, a *ϱ-flagged principal G-bundle* (*of type* $(\underline{x}, \underline{P})$) is a tuple $(\mathscr{P}, \underline{s})$ that is composed of a principal G-bundle $\mathscr{P}$ and reductions $s_i\colon \{x_i\} \longrightarrow (\mathscr{P}_{\mathrm{GL}(V)} \times_C \{x_i\})/P_i$ of the associated principal $\mathrm{GL}(V)$-bundle at the points x_i, $i = 1, ..., b$. This time, the stability parameter will be a tuple $\underline{a} = (a_1, ..., a_b)$ with $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$, $i = 1, ..., b$.
Before we introduce the correct notion of semistability, we point out that, given a parabolic subgroup Q of G, a dominant character χ on Q, and a_i as above, there is no intrinsic way to define $\langle \chi_{s_i}, a_{s_i} \rangle$ (compare Section 4). Thus, we have to explain how we extend a parabolic subgroup of G and a dominant character on it to a parabolic subgroup of $\mathrm{GL}(V)$ and a dominant character on it. For this, we use the construction introduced in [36] and [15].
Fix a basis for V and let $\widetilde{T} \subset \mathrm{GL}(V)$ be the corresponding maximal torus of diagonal matrices. The basis yields a basis for $X^\star(\widetilde{T})$, i.e., an isomorphism $X^\star(\widetilde{T}) \cong \mathbb{Z}^n$. The symmetric bilinear map $\mathbb{Z}^n \times \mathbb{Z}^n \longrightarrow \mathbb{Z}$, $((b_1, ..., b_n), (b'_1, ..., b'_m)) \longmapsto \sum_{i=1}^n b_i \cdot b'_i$ induces the symmetric bilinear map $(.,.)\colon X_\star(\widetilde{T}) \times X_\star(\widetilde{T}) \longrightarrow \mathbb{Z}$. Let $(.,.)_{\mathbb{K}}\colon X_{\star,\mathbb{K}}(\widetilde{T}) \times X_{\star,\mathbb{K}}(\widetilde{T}) \longrightarrow \mathbb{K}$ be its $\mathbb{K}$-bilinear extension to the vector space $X_{\star,\mathbb{K}}(\widetilde{T}) := X_\star(\widetilde{T}) \otimes_{\mathbb{Z}} \mathbb{K}$, $\mathbb{K} = \mathbb{Q}, \mathbb{R}$. Since the pairing $(.,.)$ is invariant under the Weyl group, it induces similar pairings on the character and cocharacter groups of any other maximal torus $\widetilde{T}' \subset \mathrm{GL}(V)$.
On the other hand, given a one-parameter subgroup $\lambda \in X_\star(\widetilde{T})$ and a character $\widetilde{\chi} \in X^\star(\widetilde{T})$, the composition $\widetilde{\chi} \circ \lambda\colon \mathbb{G}_m(k) \longrightarrow \mathbb{G}_m(k)$ is of the form $z \longmapsto z^{\langle \widetilde{\chi}, \lambda \rangle}$ and gives the duality pairing $\langle .,. \rangle\colon X^\star(\widetilde{T}) \times X_\star(\widetilde{T}) \longrightarrow \mathbb{Z}$. We let $\langle .,. \rangle_{\mathbb{K}}\colon X^\star_{\mathbb{K}}(\widetilde{T}) \times X_{\star,\mathbb{K}}(\widetilde{T}) \longrightarrow \mathbb{K}$, $\mathbb{K} = \mathbb{Q}, \mathbb{R}$, $X^\star_{\mathbb{K}}(\widetilde{T}) := X^\star(\widetilde{T}) \otimes_{\mathbb{Z}} \mathbb{K}$, be its extensions. Thus, any rational one-parameter subgroup $\lambda \in X_{\star,\mathbb{Q}}(\widetilde{T})$ gives rise to a character $\widetilde{\chi}_\lambda \in X^\star_{\mathbb{Q}}(\widetilde{T})$ defined by

$$(\lambda, \lambda')_{\mathbb{Q}} = \langle \widetilde{\chi}_\lambda, \lambda' \rangle_{\mathbb{Q}}, \quad \forall \lambda' \in X_{\star,\mathbb{Q}}(\widetilde{T}).$$

One checks that $\widetilde{\chi}_\lambda$ comes from a character of $Q := Q_{\mathrm{GL}(V)}(\lambda)$ that depends only on the conjugacy class of λ within Q. If the weighted flag of λ is, for example, $(\{0\} \subsetneq U \subsetneq V, (1))$, then

$$\begin{aligned} \widetilde{\chi}_\lambda \colon Q_{\mathrm{GL}(V)}(\lambda) &\longrightarrow \mathbb{G}_m(k) \\ \left(\begin{array}{c|c} g & \star \\ \hline 0 & h \end{array}\right) &\longmapsto \det(g)^{\dim(U)-\dim(V)} \cdot \det(h)^{\dim(U)}. \end{aligned} \tag{1}$$

If $T \subset G$ is a maximal torus, then we may extend it to a maximal torus $\widetilde{T}$ of $\mathrm{GL}(V)$. The scalar product on $X^\star_{\mathbb{K}}(\widetilde{T})$ that we have obtained before restricts to a scalar product on $X^\star_{\mathbb{K}}(T)$. Lemma 2.8 in Chapter II of [32] implies that the scalar product on $X^\star_{\mathbb{K}}(T)$ thus obtained does not depend on the choice of the extending torus $\widetilde{T}$. Furthermore, it is invariant under the Weyl group $\mathscr{N}(T)/T$.
If $\lambda\colon \mathbb{G}_m(k) \longrightarrow G$ is a one-parameter subgroup, then we associate with it the parabolic subgroup $Q_G(\lambda)$, the anti-dominant character χ_λ, and the dominant character $\chi_{-\lambda} = -\chi_\lambda$. Likewise, we have $Q_{\mathrm{GL}(V)}(\lambda)$, the anti-dominant character $\widetilde{\chi}_\lambda$, and the dominant character $\widetilde{\chi}_{-\lambda} = -\widetilde{\chi}_\lambda$. Note that $Q_G(\lambda) = Q_{\mathrm{GL}(V)}(\lambda) \cap G$ and $\widetilde{\chi}_{\pm\lambda|Q_G(\lambda)} = \chi_{\pm\lambda}$.

Proposition 5.1.1. *The assignment $\lambda \longmapsto (Q_G(\lambda), \chi_{-\lambda})$ ($\lambda \longmapsto (Q_G(\lambda), \chi_\lambda)$) is a surjection from the set of one-parameter subgroups of G onto the set of pairs consisting of a parabolic subgroup of G and a dominant (anti-dominant) character on that parabolic subgroup.*

Proof. See Section 3.2 of [15]. □

We say that a ϱ-flagged principal G-bundle $(\mathscr{P}, \underline{s})$ is *$\underline{a}$-(semi)stable*, if, for every one-parameter subgroup $\lambda\colon \mathbb{G}_m(k) \longrightarrow G$ and every reduction of $\mathscr{P}$ to the parabolic subgroup $Q := Q_G(\lambda)$, the inequality

$$\deg\bigl(\mathscr{P}_Q(\chi_{-\lambda})\bigr) + \sum_{i=1}^{b} \bigl\langle (\widetilde{\chi}_{-\lambda})_{s_i}, a_{s_i} \bigr\rangle (\le) 0$$

holds true.

Associated Flagged Principal Bundles and Semistability. — Now, we return to the situation where we are given a type $(\underline{x}, \underline{P})$ with $\underline{x}$ as usual and $\underline{P} = (P_1, ..., P_b)$ a tuple of parabolic subgroups of G and a stability parameter $\underline{a} = (a_1, ..., a_b)$ with $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$, $i = 1, ..., b$. As we have explained in Section 4, we may view a_i as a rational one-parameter subgroup of G with $P_G(a_i) = P_i$, $i = 1, ..., b$. We set $\varrho_\star(\underline{P}) := (\widetilde{P}_1, ..., \widetilde{P}_b) := (P_{\mathrm{GL}(V)}(a_1), ..., P_{\mathrm{GL}(V)}(a_b))$ and $\varrho_\star(\underline{a}) := (\widetilde{a}_1, ..., \widetilde{a}_b) := (\varrho \circ a_1, ..., \varrho \circ a_s)$. Next note that any flagged principal G-bundle $(\mathscr{P}, \underline{s})$ of type $(\underline{x}, \underline{P})$ defines the ϱ-flagged principal $\mathrm{GL}(V)$-bundle $(\mathscr{P}_{\mathrm{GL}(V)}, \varrho_\star(\underline{s}))$, $\varrho_\star(\underline{s}) = (\widetilde{s}_1, ..., \widetilde{s}_b)$, with

$$\widetilde{s}_i \colon \{x_i\} \xrightarrow{s_i} \mathscr{P}_{|\{x_i\}}/P_i \hookrightarrow \mathscr{P}_{\mathrm{GL}(V)|\{x_i\}}/\widetilde{P}_i, \quad i = 1, ..., b.$$

Lemma 5.1.2. *A flagged principal G-bundle $(\mathscr{P}, \underline{s})$ of type $(\underline{x}, \underline{P})$ is $\underline{a}$-(semi)stable, if and only if the associated ϱ-flagged principal* $\mathrm{GL}(V)$*-bundle* $(\mathscr{P}_{\mathrm{GL}(V)}, \varrho_\star(\underline{s}))$ *of type* $(\underline{x}, \varrho_\star(\underline{P}))$ *is* $\varrho_\star(\underline{a})$*-(semi)stable.*

Proof. By Proposition 5.1.1, $(\mathscr{P}, \underline{s})$ is $\underline{a}$-(semi)stable, if and only if, for every one-parameter subgroup $\lambda\colon \mathbb{G}_m(k) \longrightarrow G$ and every reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to $Q := Q_G(\lambda)$, one has

$$\deg\bigl(\mathscr{P}_Q(\chi_{-\lambda})\bigr) + \sum_{i=1}^{b}\bigl\langle(\chi_{-\lambda})_{s_i}, a_{s_i}\bigr\rangle(\leq)0.$$

Our contention therefore reduces to the trivial fact $\langle(\chi_{-\lambda})_{s_i}, a_{s_i}\rangle = \langle(\widetilde{\chi}_{-\lambda})_{s_i}, \widetilde{a}_{s_i}\rangle$, $i = 1, ..., b$. □

Another Formulation of Semistability for ϱ-Flagged Principal Bundles. — Before we may introduce even more general objects, we have to reformulate the notion of $\underline{a}$-(semi)stability. The first trivial reformulation is that we may say that $(\mathscr{P}, \underline{s})$ is $\underline{a}$-(semi)stable, if, for every one-parameter subgroup $\lambda\colon \mathbb{G}_m(k) \longrightarrow G$ and every reduction of $\mathscr{P}$ to the parabolic subgroup $Q := Q_G(\lambda)$, the inequality

$$\deg\bigl(\mathscr{P}_Q(\chi_\lambda)\bigr) + \sum_{i=1}^{b}\bigl\langle(\widetilde{\chi}_\lambda)_{s_i}, a_{s_i}\bigr\rangle(\geq)0$$

holds true.

Next, assume we are given a principal G-bundle $\mathscr{P}$, a one-parameter subgroup $\lambda\colon \mathbb{G}_m(k) \longrightarrow G$ with weighted flag

$$\bigl(V_\bullet(\lambda), \beta_\bullet(\lambda)\bigr) = \bigl(\{0\} \subsetneq V_1 \subsetneq \cdots \subsetneq V_t \subsetneq V, (\beta_1, ..., \beta_t)\bigr),$$

and a reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to $Q := Q_G(\lambda)$. Then, we obtain an induced reduction $\mathscr{P}_{Q_{\mathrm{GL}(V)}(\lambda)}$ of the principal $\mathrm{GL}(V)$-bundle $\mathscr{P}_{\mathrm{GL}(V)}$ to $Q_{\mathrm{GL}(V)}(\lambda)$. The datum of that reduction is equivalent to the datum of a filtration

$$E_\bullet(\mathscr{P}_Q) : \{0\} \subsetneq E_1 \subsetneq \cdots \subsetneq E_t \subsetneq E \quad \text{with } \mathrm{rk}(E_i) = \dim(V_i),\ i = 1, ..., t.$$

Using (1), one easily computes

$$\deg\bigl(\mathscr{P}_Q(\chi_\lambda)\bigr) = \sum_{i=1}^{t}\beta_i \cdot \bigl(\deg(E)\cdot \mathrm{rk}(E_i) - \deg(E_i)\cdot \mathrm{rk}(E)\bigr). \tag{2}$$

Note that a parabolic subgroup of $\mathrm{GL}(V)$ is the stabilizer of a flag in V. Thus, the tuple $\underline{P}$ of parabolic subgroups of $\mathrm{GL}(V)$ gives quotients $V \longrightarrow W_{ij}$, and subspaces $V_{ij} := \ker(V \longrightarrow W_{ij})$, $j = 1, ..., t_i$, $i = 1, ..., b$, such that $V_{ij} \subsetneq V_{ij+1}$, $j = 1, ..., t_i - 1$, $i = 1, ..., b$.

Next, let $\lambda\colon \mathbb{G}_m(k) \longrightarrow G$ be a one-parameter subgroup with weighted flag

$$\big(V_\bullet(\lambda), \beta_\bullet(\lambda)\big) = \big(\{0\} \subsetneq V_1' \subsetneq \cdots \subsetneq V_t' \subsetneq V, (\beta_1, ..., \beta_t)\big)$$

and a a rational one-parameter subgroup of G with weighted flag

$$\big(V_\bullet(a), \beta_\bullet(a)\big) = \left(\{0\} \subsetneq V_1 \subsetneq \cdots \subsetneq V_\tau \subsetneq V, \frac{1}{\dim(V)} \cdot (a_1, ..., a_\tau)\right).$$

In addition, define

$$Q_h := V/V_h, \quad R_{ih} := V_i'/(V_i' \cap V_h), \quad r_{ih} := \dim(R_{ih}), \quad i = 1, ..., t, h = 1, ..., \tau,$$

$r := \dim(V)$. We claim that

$$\langle \widetilde{\chi}_\lambda, a\rangle = \sum_{i=1}^{t} \Big(\beta_i \cdot \sum_{h=1}^{\tau} a_h \cdot \big(r \cdot r_{ih} - r_j \cdot \dim(Q_h)\big)\Big). \tag{3}$$

By bilinearity, this has to be checked only for $\tau = t = 1$, $\beta_1 = 1$, and $a_1 = r$. In this case, it follows easily from the definitions and (1).
Finally, suppose we are given a stability parameter $\underline{a} = (a_1, ..., a_b)$ with $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$, $i = 1, ..., b$. Then, we write $\beta_\bullet(a_i) =: (1/r)\cdot(a_{i1}, ..., a_{it_i})$, $i = 1, ..., b$. The parabolic subgroups $P_1, ..., P_b$ define quotients $V \longrightarrow W_{ij}$, and we set $r_{ij} := \dim(W_{ij})$, $j = 1, ..., t_i$, $i = 1, ..., b$. Suppose that $(\mathscr{P}, \underline{s})$ is a ϱ-flagged principal G-bundle of type $(\underline{x}, \underline{P})$. Then, we have the associated vector bundle E, and the reductions s_i define quotients $q_{ij}\colon E_i \longrightarrow Q_{ij}$ with $\dim(Q_{ij}) = r_{ij}$, $j = 1, ..., t_i$, $i = 1, ..., b$. For any subbundle $\{0\} \subsetneq F \subsetneq E$, we set

$$\underline{a}\text{-}\deg(F) := \deg(F) - \sum_{i=1}^{b}\sum_{j=1}^{t_i} a_{ij} \cdot \dim\big(q_{ij}(F)\big).$$

Putting (2) and (3) together, we infer the following characterization of semistability.

Proposition 5.1.3. *The ϱ-flagged principal G-bundle is $\underline{a}$-(semi)stable, if and only if, for every one-parameter subgroup λ of G and every reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to $Q := Q_G(\lambda)$, the inequality*

$$\sum_{i=1}^{t} \beta_i\big(\underline{a}\text{-}\deg(E) \cdot \mathrm{rk}(E_i) - \underline{a}\text{-}\deg(E_i) \cdot \mathrm{rk}(E)\big)(\geq)0$$

is verified. Here,

$$E_\bullet\big(\mathscr{P}_Q\big) = \{0\} \subsetneq E_1 \subsetneq \cdots \subsetneq E_t \subsetneq E \quad \textit{and} \quad \beta_\bullet(\lambda) = (\beta_1, ..., \beta_t).$$

Reminder on Pseudo G-Bundles. — Following the general strategy from [36] and [15], we will first embed principal G-bundles into pseudo G-bundles which in turn can be embedded into decorated vector bundles for which we finally can do the GIT-calculations. We have already chosen to view principal G-bundles as principal $\mathrm{GL}(V)$-bundles together with a reduction to G, i.e., as pairs $(\mathscr{P},\sigma)$ that consist of a principal $\mathrm{GL}(V)$-bundle $\mathscr{P}$ and a section $\sigma\colon C\longrightarrow \mathscr{P}/G$. Given such a pair $(\mathscr{P},\sigma)$, let E be the corresponding vector bundle. Then,

$$\mathscr{P}=\mathscr{I}\!som(V\otimes\mathscr{O}_C,E)\subset\mathscr{H}\!om(V\otimes\mathscr{O}_C,E)=\mathrm{Spec}\big(\mathscr{S}\!ym^\star(V\otimes E^\vee)\big).$$

Moreover, the good quotient $\mathscr{H}\!om(V\otimes\mathscr{O}_C,E)/\!\!/G=\mathrm{Spec}(\mathscr{S}\!ym^\star(V\otimes E)^G)$ exists and there is the open embedding

$$\mathscr{I}\!som(V\otimes\mathscr{O}_C,E)/G\subset\mathscr{H}\!om(V\otimes\mathscr{O}_C,E)/\!\!/G.$$

Thus, σ is given by a non-trivial homomorphism $\tau\colon\ \mathscr{S}\!ym^\star(V\otimes E^\vee)^G\longrightarrow\mathscr{O}_C$. This suggests the following definition: a *pseudo G-bundle* (E,τ) consists of a vector bundle E with trivial determinant $\det(E)\cong\mathscr{O}_C$ and a non-trivial homomorphism $\tau\colon\ \mathscr{S}\!ym^\star(V\otimes E^\vee)^G\longrightarrow\mathscr{O}_C$ of $\mathscr{O}_C$-algebras. Not any homomorphism τ gives rise to a principal G-bundle, but the following result ([36], Corollary 3.4) gives an important characterization when it does.

Lemma 5.1.4. *Let (E,τ) be a pseudo G-bundle with associated section $\sigma\colon C\longrightarrow \mathscr{H}\!om(V\otimes\mathscr{O}_C,E)/\!\!/G$. Then, (E,τ) is a principal G-bundle, if and only if there exists a point $x\in C$, such that*

$$\sigma(x)\in\mathrm{Isom}(V,E_{|\{x\}})/G.$$

For our purposes, we therefore look at the following objects: a *ϱ-flagged pseudo G-bundle* $(E,\tau,\underline{q})$ is a pseudo G-bundle (E,τ) together with quotients

$$q_{ij}\colon E_{|\{x_i\}}\longrightarrow Q_{ij}$$

onto k-vector spaces Q_{ij}, $j=1,...,t_i$, $i=1,...,b$, such that

$$\ker(q_{ij})\subseteq\ker(q_{ij+1}),\quad j=1,...,t_i-1,i=1,...,b.\tag{4}$$

The tuple $(\underline{x},\underline{r})$ with $\underline{r}=(r_{ij}:=\dim(Q_{ij}),j=1,...,t_i,i=1,...,s)$ will be referred to as the *type of the flagging.* There is an obvious notion of *isomorphism of ϱ-flagged pseudo G-bundles.*

The algebra $\mathscr{S}\!ym^\star(V\otimes E^\vee)^G$ is finitely generated, so that the morphism τ is determined, for $s\gg 0$, by its restriction $\tau_{\le s}\colon\ \bigoplus_{i=1}^s\mathscr{S}\!ym^i(V\otimes E^\vee)^G\longrightarrow\mathscr{O}_C$. In particular, ϱ-flagged pseudo-G-bundles form an algebraic stack, locally of finite type. Lemma 5.1.4 implies that the stack of ϱ-flagged G-bundles is an open substack of the stack of ϱ-flagged pseudo G-bundles. Following [15], we choose $s\gg 0$, such that

a) $\mathrm{Sym}^\star(V\otimes k^{r\vee})^G$ is generated by elements in degree $\leq s$.

b) $\mathrm{Sym}^{(s!)}(V\otimes k^{r\vee})^G$ is generated by elements in degree 1, i.e., by the elements in the vector space $\mathrm{Sym}^{s!}(V\otimes k^{r\vee})^G$.

Set

$$\mathbb{V}_s(E):=\bigoplus_{\substack{(d_1,\ldots,d_s):\\ d_i\geq 0,\sum id_i=s!}}\Big(\mathrm{Sym}^{d_1}\big((V\otimes E^\vee)^G\big)\otimes\cdots\otimes\mathrm{Sym}^{d_s}\big(\mathrm{Sym}^s(V\otimes E^\vee)^G\big)\Big).$$

Then, τ induces morphisms

$$\tau^{s!}\colon \mathscr{S}ym^{s!}(V\otimes E^\vee)^G\longrightarrow \mathscr{O}_C$$

and

$$\varphi\colon \mathbb{V}_s(E)\twoheadrightarrow \mathscr{S}ym^{s!}(V\otimes E^\vee)^G\longrightarrow \mathscr{O}_C.$$

Homogeneous Representations. — Instead of the representation $\mathbb{V}_s$, we can also allow a more general class of representations without complicating the arguments. This might be useful for other applications, too. A representation $\kappa\colon \mathrm{GL}_r(k)\longrightarrow \mathrm{GL}(U)$ is called a *polynomial representation*, if it extends to a (multiplicative) map $\overline{\kappa}\colon M_r(k)\longrightarrow \mathrm{End}(U)$. We say that κ is *homogeneous of degree* $u\in\mathbb{Z}$, if

$$\kappa\big(z\cdot\mathbb{E}_r\big)=z^u\cdot\mathrm{id}_U,\quad \forall z\in\mathbb{G}_m(k).$$

Let $P(r,u)$ be the abelian category of homogeneous polynomial representations of $\mathrm{GL}_r(k)$ of degree u. It comes with the duality functor

$$\begin{array}{rccc} {}^\star\colon & P(r,u) & \longrightarrow & P(r,u)\\ & \kappa & \longmapsto & \big(\kappa\circ\mathrm{id}^\vee_{\mathrm{GL}_r(k)}\big)^\vee. \end{array}$$

Here, $.^\vee$ stands for the corresponding dual representation. An example for a representation in $P(r,u)$ is the *u-th divided power* $(\mathrm{Sym}^u(\mathrm{id}_{\mathrm{GL}_r(k)}))^\star$, i.e., the representation of $\mathrm{GL}_r(k)$ on

$$D^u(W):=\big(\mathrm{Sym}^u(W^\vee)\big)^\vee,\quad W:=k^r.$$

More generally, we look, for $u,v>0$, at the $\mathrm{GL}_r(k)$-module

$$\mathbb{D}^{u,v}(W):=\bigoplus_{\substack{(u_1,\ldots,u_v):\\ u_i\geq 0,\sum_{i=1}^v u_i=u}}\big(D^{u_1}(W)\otimes\cdots\otimes D^{u_v}(W)\big). \tag{5}$$

Lemma 5.1.5. *Let* $\kappa\colon \mathrm{GL}_r(k)\longrightarrow\mathrm{GL}(U)$ *be a homogeneous polynomial representation of degree* u. *Then, there exists an integer* $v>0$, *such that* U *is a quotient of the* $\mathrm{GL}(U)$*-module* $\mathbb{D}^{u,v}(W)$. *If* κ *is homogeneous, but not polynomial, then it is a quotient of* $\mathbb{D}^{u,v}(W)\otimes(\bigwedge^r W)^{\otimes -w}$ *for some* $w>0$.

Proof. The proof of Proposition 5.3 in [27] shows that any representation $\kappa'\colon \mathrm{GL}_r(k) \longrightarrow \mathrm{GL}(U')$ in $P(r,u)$ is, for suitable $v>0$, a sub-representation of the representation of $\mathrm{GL}_r(k)$ on the vector space

$$\bigoplus_{\substack{(u_1,\dots,u_v):\\ u_i\geq 0,\sum_{i=1}^v u_i=u}} \bigl(\mathrm{Sym}^{u_1}(W)\otimes\cdots\otimes\mathrm{Sym}^{u_v}(W)\bigr).$$

Applying this result to the dual $\kappa^\star\colon \mathrm{GL}_r(k)\longrightarrow \mathrm{GL}(U^\star)$ of κ proves the first assertion.
The second assertion follows from the obvious fact that $U\otimes(\bigwedge^r W)^{\otimes w}$ will be a polynomial representation for large w. □

Remark 5.1.6. As is apparent from the construction in [27], the above result also holds over the ring of integers.

Fix natural numbers u,v and let A be any vector bundle on the curve C, that is, we do not assume A to have rank r. Then, we set for $w\geq 0$

$$\mathbb{D}^{u,v}(A) := \bigoplus_{\substack{(u_1,\dots,u_v):\\ u_i\geq 0,\sum_{i=1}^v u_i=u}} \bigl(D^{u_1}(A)\otimes\cdots\otimes D^{u_v}(A)\bigr),\quad D^w(A) := \bigl(\mathscr{S}\!ym^w(A^\vee)\bigr)^\vee.$$

Remark 5.1.7. Any surjective homomorphism $\psi\colon A\longrightarrow B$ between vector bundles induces a surjective homomorphism

$$\mathbb{D}^{u,v}(\psi)\colon \mathbb{D}^{u,v}(A)\longrightarrow \mathbb{D}^{u,v}(B).$$

Decorated Flagged Vector Bundles. — Now, fix a line bundle L on C. A *decorated flagged vector bundle of type* $(r,d,\underline{x},\underline{r},u,v,L)$ is a tuple $(E,\underline{q},\varphi)$ which consists of a vector bundle E on C of rank r and degree d, a non-trivial homomorphism

$$\varphi\colon \mathbb{D}^{u,v}(E)\longrightarrow L,$$

and a flagging $\underline{q}=(q_{ij}\colon E_{|\{x_i\}}\longrightarrow Q_{ij}, j=1,\dots,t_i, i=1,\dots,s)$ of type $\underline{r}=(r_{ij}, j=1,\dots,t_i, i=1,\dots,s)$. The moduli functors for the objects we have considered, so far, are straightforward to define (just form the isomorphism classes in the corresponding stack). For decorated flagged vector bundles, this is slightly more delicate. Thus, we give the definition. A *family of decorated flagged vector bundles of type* $(r,d,\underline{x},\underline{r},u,v,L)$ (*parameterized by the scheme* S) is a tuple $(E_S,\underline{q}_S,\mathscr{N}_S,\varphi_S)$ which consists of a vector bundle E_S of rank r on $S\times C$ and fiberwise of degree d, a tuple $\underline{q}_S=(q_{S,ij}\colon E_{S|S\times\{x_i\}}\longrightarrow Q_{S,ij})$ of surjections onto vector bundles $Q_{S,ij}$ of rank r_{ij}, $j=1,\dots,t_i$, $i=1,\dots,b$, subject to the conditions in (4), a line bundle $\mathscr{N}_S$ on S, and a homomorphism $\varphi_S\colon \mathbb{D}^{u,v}(E_S)\longrightarrow \pi_C^\star(L)\otimes\pi_S^\star(\mathscr{N}_S)$ which is non-trivial on every fiber $\{s\}\times C$. Two such families $(E_S,\underline{q}_S,\mathscr{N}_S,\varphi_S)$ and $(E'_S,\underline{q}'_S,\mathscr{N}'_S,\varphi'_S)$ are said to be *isomorphic*, if there exist isomorphisms $\psi_S\colon E_S\longrightarrow E'_S$ and $\chi_S\colon \mathscr{N}_S\longrightarrow\mathscr{N}'_S$ fulfilling

$$q_{S,ij}=q'_{S,ij}\circ\psi_{S|S\times\{x_i\}},\quad j=1,\dots,t_i,\ i=1,\dots,b,$$

and

$$\varphi_S = \left(\mathrm{id}_{\pi_C^\star(L)} \otimes \pi_S^\star(\chi_S)\right)^{-1} \circ \varphi_S' \circ \mathbb{D}^{u,v}(\psi_S).$$

Thus, we may form the functor that assigns to every scheme the set of isomorphism classes of families of decorated vector bundles of type $(r, d, \underline{x}, \underline{r}, u, v, L)$ parameterized by S.

By Lemma 5.1.5, the representation $\mathbb{V}_s$ can be written as the quotient of $\mathbb{D}^{u,v}(W) \otimes (\bigwedge^r W)^{\otimes -s!}$. Now, suppose we are given a vector bundle E_S on $S \times C$, a homomorphism $\tau_S \colon \mathscr{S}ym^\star(V \otimes E_S^\vee)^G \longrightarrow \mathscr{O}_{S\times C}$ and a flagging $\underline{q}_S$ of type $(\underline{x}, \underline{r})$ of E_S. Then, the determinant of E_S is isomorphic to the pullback of a line bundle $\mathscr{D}_S$ on S. Choose an isomorphism $\det(E_S) \cong \pi_S^\star(\mathscr{D}_S)$, and set $\mathscr{N}_S := \mathscr{D}^{\otimes s!}$, so that τ_S gives rise to

$$\mathbb{D}^{u,v}(E_S) \otimes \mathscr{N}_S^\vee \twoheadrightarrow \mathbb{V}_s(E_S) \twoheadrightarrow \mathscr{S}ym^{s!}(V \otimes E_S^\vee)^G \longrightarrow \mathscr{O}_{S\times C}.$$

Thus, we obtain the family $(E_S, \underline{q}_S, \mathscr{N}_S, \varphi_S)$ of decorated flagged vector bundles. Its isomorphism class does not depend on the choice of the isomorphism $\det(E_S) \cong \pi_S^\star(\mathscr{D}_S)$, so that this construction gives rise to a natural transformation of functors.

Lemma 5.1.8. *The above natural transformation applied to $S = \mathrm{Spec}(K)$, K an algebraically closed extension of k, is injective.*

Proof. The proof is the same as the one of Lemma 5.1.1 in [15]. □

We now come to the definition of semistability. Fix the stability parameter $\underline{a}$ for the flagging. Here, we view $\underline{a} = (a_{ij}, j = 1, ..., t_i, i = 1, ..., s)$ as a tuple of rational numbers, and we assume that

- $a_{ij} > 0$, $j = 1, ..., t_i$, $i = 1, ..., s$;
- $\sum_{j=1}^{t_i} a_{ij} < 1$, $i = 1, ..., s$.

Then, given a decorated flagged vector bundle $(E, \underline{q}, \varphi)$ and a weighted filtration $(E_\bullet, \beta_\bullet)$ of E, we define

$$M_{\underline{a}}(E_\bullet, \beta_\bullet) := \sum_{j=1}^{t} \beta_j \cdot \left(\underline{a}\text{-}\deg(E) \cdot \mathrm{rk}(E_j) - \underline{a}\text{-}\deg(E_j) \cdot \mathrm{rk}(E)\right).$$

The quantity $\mu(E_\bullet, \beta_\bullet; \varphi)$ is obtained as follows. Let η be the generic point of the curve C and let $\mathbb{E}$ stand for the restriction of E to $\{\eta\}$. Then, the restricted homomorphism $\varphi_{|\{\eta\}}$ gives a point

$$\sigma_\eta \in \mathbb{P}\left(\mathbb{D}^{u,v}(\mathbb{E})\right).$$

We may choose a one-parameter subgroup $\lambda_K \colon \mathbb{G}_m(K) \longrightarrow \mathrm{SL}(\mathbb{E})$, $K := k(C)$, whose weighted flag agrees with the restriction of $(E_\bullet, \beta_\bullet)$ to $\{\eta\}$ and define

$$\mu\left(E_\bullet, \beta_\bullet; \varphi\right) := \mu(\lambda_K, \sigma_\eta).$$

This does not depend on the choice of λ_K.

Remark 5.1.9. By construction, the vector bundle $\mathbb{D}^{u,v}(E)$ is a subbundle of $(E^{\otimes u})^{\oplus N}$ for some $N > 0$. Set $E_{t+1} := E$ and, for $(i_1, ..., i_u) \in \{1, ..., t+1\}^{\times u}$,

$$E_{i_1} \star \cdots \star E_{i_u} := \big(E_{i_1} \otimes \cdots \otimes E_{i_u}\big)^{\oplus N} \cap \mathbb{D}^{u,v}(\mathbb{E}).$$

For a weighted filtration $(E_\bullet, \beta_\bullet)$ of the vector bundle E, we define the *associated (integral) weight vector*

$$\big(\underbrace{\gamma_1, \ldots, \gamma_1}_{(\operatorname{rk} E_1)\times}, \underbrace{\gamma_2, \ldots, \gamma_2}_{(\operatorname{rk} E_2 - \operatorname{rk} E_1)\times}, \ldots, \underbrace{\gamma_{t+1}, \ldots, \gamma_{t+1}}_{(\operatorname{rk} E - \operatorname{rk} E_t)\times}\big) := \sum_{l=1}^{t} \beta_l \cdot \gamma_r^{(\operatorname{rk} E_l)}. \tag{6}$$

(Note that we recover $\beta_l = (\gamma_{l+1} - \gamma_l)/r$, $l = 1, ..., t$.)
With these concepts, one readily verifies

$$\mu\big(E_\bullet, \beta_\bullet; \varphi\big) = \\ -\min\Big\{\, \gamma_{i_1} + \cdots + \gamma_{i_u} \,\big|\, (i_1, ..., i_u) \in \{1, ..., t+1\}^{\times u} : \varphi_{|(E_{i_1} \star \cdots \star E_{i_u})} \not\equiv 0 \Big\}.$$

To define semistability, we also fix a positive rational number δ. Then, we say that a decorated flagged vector bundle is $(\underline{a}, \delta)$-*(semi)stable*, if the inequality

$$M_{\underline{a}}(E_\bullet, \beta_\bullet) + \delta \cdot \mu\big(E_\bullet, \beta_\bullet; \varphi\big)(\geq)0$$

holds for any weighted filtration $(E_\bullet, \beta_\bullet)$ of E.

Boundedness. — The starting point for the GIT construction is the boundedness of the family of $(\underline{a}, \delta)$-semistable decorated flagged vector bundles of type $(r, d, \underline{x}, \underline{r}, u, v, L)$. This property is a consequence of the following statement.

Proposition 5.1.10. *Fix the type $(r, d, \underline{x}, \underline{r}, u, v, L)$ and the stability parameter δ. Then, there is a positive constant D_0, such that, given a tuple $\underline{a} = (a_{ij}, j = 1, ..., t_i, 1 = 1, ..., s)$ of positive rational numbers with $\sum_{j=1}^{t_i} a_{ij} < 1$ for $i = 1, ..., s$ and an $(\underline{a}, \delta)$-semistable decorated flagged vector bundle $(E, \underline{q}, \varphi)$ of type $(r, d, \underline{x}, \underline{r}, u, v, L)$, one finds*

$$\mu_{\max}(E) \leq \frac{d}{r} + D_0.$$

Proof. Let $(F, \underline{\widetilde{q}})$ be any vector bundle with a flagging of type $\underline{r}$. Setting $R := \max\{ r_{ij} \,|\, j = 1, ..., t_i, i = 1, ..., s \}$, we derive, for $\underline{a}$ as in the proposition, the obvious estimate

$$\deg(F) \geq \underline{a}\text{-}\deg(F) \geq \deg(F) - s \cdot R.$$

Now, let $(E, \underline{q}, \varphi)$ be as above and $0 \subsetneq F \subsetneq E$ a subbundle. For the weighted filtration $(E_\bullet : 0 \subsetneq F \subsetneq E, \beta_\bullet = (1))$, one checks

$$\mu(E_\bullet, \beta_\bullet; \varphi) \leq u \cdot (r - 1).$$

Together with these two estimates, the condition of $(\underline{a},\delta)$-semistability implies

$$\begin{aligned} d\cdot \mathrm{rk}(F) - \deg(F)\cdot r + s\cdot r\cdot R + \delta\cdot u\cdot (r-1) \\ \geq \underline{a}\text{-}\deg(E)\cdot \mathrm{rk}(F) - \underline{a}\text{-}\deg(F)\cdot r + \delta\cdot \mu(E_\bullet,\beta_\bullet;\varphi) \geq 0. \end{aligned}$$

We transform this into the inequality

$$\mu(F) \leq \frac{d}{r} + \frac{s\cdot r\cdot R + \delta\cdot u\cdot (r-1)}{\mathrm{rk}(F)\cdot r} \leq \frac{d}{r} + \underbrace{s\cdot R + \frac{\delta\cdot u\cdot (r-1)}{r}}_{=:D_0}.$$

This is the assertion we made. □

5.2 The Moduli Space of Decorated Flagged Vector Bundles

Suppose we are given a constant D. Then, we let $\mathfrak{S}$ be the bounded family of isomorphism classes of vector bundles of rank r and degree d with $\mu_{\max}(E) \leq D$. We also fix an ample line bundle $\mathscr{O}_C(1)$ of degree one on C, a natural number n, such that $E(n)$ is globally generated and $H^1(E(n)) = \{0\}$ for any vector bundle E, such that $[E] \in \mathfrak{S}$, as well as a vector space Y of dimension $d + r(n+1-g)$. Now, a *quotient family of decorated flagged vector bundles of type* $(r,d,\underline{x},\underline{r},u,v,L)$ (*parameterized by the scheme* S) is a tuple $(k_S,\underline{q}_S,\mathscr{N}_S,\varphi_S)$ which consists of a quotient $k_S\colon Y\otimes \pi_C^\star(\mathscr{O}_C(n)) \longrightarrow E_S$, a tuple $\underline{q}_S = (q_{S,ij}\colon E_{S|S\times\{x_i\}} \longrightarrow Q_{S,ij}, j=1,...,t_i, i=1,...,b)$, a line bundle $\mathscr{N}_S$ on S, and a homomorphism $\varphi_S\colon \mathbb{D}^{u,v}(E_S) \longrightarrow \pi_C^\star(L)\otimes \pi_S^\star(\mathscr{N}_S)$ with the following properties:

- E_S is a vector bundle on $S\times C$, such that $[E_{S|\{s\}\times C}] \in \mathfrak{S}$, for every $s\in S(k)$,
- $\pi_{S\star}(k_S\otimes \mathrm{id}_{\pi_C^\star(\mathscr{O}_C(n))})\colon Y\otimes \mathscr{O}_S \longrightarrow \pi_{S\star}(E_S\otimes \pi_C^\star(\mathscr{O}_C(n)))$ is an isomorphism,
- $\underline{q}_S$ consists of surjections onto vector bundles $Q_{S,ij}$ of rank r_{ij}, $j = 1,...,t_i$, $i=1,...,b$, subject to the conditions in (4), and
- φ_S is non-trivial on every fiber $\{s\}\times C$.

Two such families $(k_S,\underline{q}_S,\mathscr{N}_S,\varphi_S)$ and $(k'_S,\underline{q}'_S,\mathscr{N}'_S,\varphi'_S)$ are said to be *isomorphic*, if there exist isomorphisms $\psi_S\colon E_S \longrightarrow E'_S$ and $\chi_S\colon \mathscr{N}_S \longrightarrow \mathscr{N}'_S$, fulfilling

$$k_S = k'_S\circ\psi_S,\ q_{S,ij} = q'_{S,ij}\circ \psi_{S|S\times\{x_i\}},\ j=1,...,t_i, i=1,...,b,$$

$$\varphi_S = \left(\mathrm{id}_{\pi_C^\star(L)}\otimes \pi_S^\star(\chi_S)\right)^{-1}\circ\varphi'_S\circ \mathbb{D}^{u,v}(\psi_S).$$

Suppose we are also given stability parameters $\underline{a}$ and δ as above. Then, we take $D = D_0$ from Proposition 5.1.10. The first step toward the construction of the moduli spaces is the construction of a suitable parameter space:

Proposition 5.2.1. *Fix the input data* $(r, d, \underline{x}, \underline{r}, u, v, L)$, *and let* D_0 *be a before. Then, the functor that assigns to a scheme* S *the set of isomorphism classes of quotient families of type* $(r, d, \underline{x}, \underline{r}, u, v, L)$ *is representable by a quasi-projective scheme* $\mathfrak{P}$.

By its universal property, the parameter scheme $\mathfrak{P}$ comes with a natural action of $\mathrm{GL}(Y)$. The next theorem is the main GIT-result that we will prove.

Theorem 5.2.2. i) *There are open subschemes* $\mathfrak{P}^{(\underline{a},\delta)\text{-(s)s}}$ *whose* k*-rational points are the classes of tuples* $(q\colon Y \otimes \mathscr{O}_C(-n) \longrightarrow E, \underline{q}, \varphi)$, *such that* $(E, \underline{q}, \varphi)$ *is an* $(\underline{a}, \delta)$*-(semi)stable decorated flagged vector bundle of type* $(r, d, \underline{x}, \underline{r}, u, v, L)$.
ii) *The good quotient*

$$\mathscr{M}(r, d, \underline{x}, \underline{r}, u, v, L)^{(\underline{a},\delta)\text{-ss}} := \mathfrak{P}^{(\underline{a},\delta)\text{-ss}} /\!\!/ \mathrm{GL}(Y)$$

exists as a projective scheme over $\mathrm{Spec}(k)$, *and the geometric quotient*

$$\mathscr{M}(r, d, \underline{x}, \underline{r}, u, v, L)^{(\underline{a},\delta)\text{-s}} := \mathfrak{P}^{(\underline{a},\delta)\text{-s}} / \mathrm{GL}(Y)$$

as an open subscheme of $\mathscr{M}(r, d, \underline{x}, \underline{r}, u, v, L)^{(\underline{a},\delta)\text{-ss}}$.

Let $\mathrm{M}(r, d, \underline{x}, \underline{r}, u, v, L)^{(\underline{a},\delta)\text{-(s)s}}$ stand for the functor that associates with a scheme S the set of isomorphism classes of families of $(\underline{a}, \delta)$-(semi)stable decorated flagged vector bundles of type $(r, d, \underline{x}, \underline{r}, u, v, L)$ parameterized by S. We infer from the above theorem:

Corollary 5.2.3. *The scheme* $\mathscr{M}(r, d, \underline{x}, \underline{r}, u, v, L)^{(\underline{a},\delta)\text{-(s)s}}$ *is the coarse moduli scheme for the functor* $\mathrm{M}(r, d, \underline{x}, \underline{r}, u, v, L)^{(\underline{a},\delta)\text{-(s)s}}$.

Remark 5.2.4. The divided powers are clearly defined over the integers. Therefore, the above theorem also works in the relative setting, i.e., for a curve $\mathscr{C} \longrightarrow \mathrm{Spec}(R)$, possessing a section. The justification has already been given in Remark 3.2.4.

Now that we have stated our main result on the moduli spaces of decorated flagged vector bundles and have explained how we get from flagged principal G-bundles to decorated flagged vector bundles, we must next show how to work our way back from the above theorem to get moduli spaces of flagged principal G-bundles. This will be the content of the next sections.

5.3 The Moduli Space for ϱ-Flagged Pseudo G-Bundles

Let D, $\mathfrak{S}$, n, and Y be as above. A *quotient family of* ϱ*-flagged pseudo* G*-bundles of type* $(\underline{x}, \underline{r})$ (*parameterized by the scheme* S) is a tuple $(k_S, \tau_S, \underline{q}_S)$ which is composed of a quotient $k_S\colon Y \otimes \pi_C^\star(\mathscr{O}_C(n)) \longrightarrow E_S$, a homomorphism $\tau_S\colon \mathscr{S}ym^\star(V \otimes E_S^\vee) \longrightarrow \mathscr{O}_{S\times C}$, and a tuple $\underline{q}_S = (q_{S,ij}\colon E_{S|S\times\{x_i\}} \longrightarrow Q_{S,ij}, j = 1, ..., t_i, i = 1, ..., b)$, such that

- E_S is a vector bundle on $S \times C$, such that $[E_{S|\{s\}\times C}] \in \mathfrak{S}$, for every $s \in S(k)$,
- $\pi_{S\star}(k_S \otimes \mathrm{id}_{\pi_C^\star(\mathscr{O}_C(n))})\colon Y \otimes \mathscr{O}_S \longrightarrow \pi_{S\star}(E_S \otimes \pi_C^\star(\mathscr{O}_C(n)))$ is an isomorphism, and
- τ_S is non-trivial on every fiber $\{s\} \times C$.

For these quotient families, we have an obvious notion of *isomorphism*.

Proposition 5.3.1. *Fix the input data D and $(\underline{x}, \underline{r})$. The functor that assigns to a scheme S the set of isomorphism classes of quotient families of ϱ-flagged pseudo G-bundles of type $(\underline{x}, \underline{r})$ is representable by a quasi-projective scheme $\mathfrak{F}_{\varrho\text{-FLPsBun}}$.*
Let $\mathfrak{Q}$ be the quasi-projective scheme that parameterizes quotients $q\colon Y \otimes \mathscr{O}_C(-n) \longrightarrow E$, such that $[E] \in \mathfrak{S}$ and $H^0(q(n))$ is an isomorphism. The natural morphism $\mathfrak{F}_{\varrho\text{-FLPsBun}} \longrightarrow \mathfrak{Q}$ induces a projective morphism $\mathfrak{F}_{\varrho\text{-FLPsBun}}/\!\!/\mathbb{G}_m(k) \longrightarrow \mathfrak{Q}$. (Here, the $\mathbb{G}_m(k)$-action comes from the embedding of $\mathbb{G}_m(k)$ into $\mathrm{GL}(Y)$ as the group of homotheties and the natural $\mathrm{GL}(Y)$-action on $\mathfrak{F}_{\varrho\text{-FLPsBun}}$.)

Fix stability parameters $\underline{a}$ and δ as before. We say that a ϱ-flagged pseudo G-bundle $(E, \tau, \underline{q})$ is $(\underline{a}, \delta)$-*(semi)stable*, if the associated decorated flagged vector bundle $(E, \underline{q}, \varphi)$ is so. Given the type $(\underline{x}, \underline{r})$, we define the moduli functor $\mathrm{M}(\varrho, \underline{x}, \underline{r})^{(\underline{a},\delta)\text{-(s)s}}$ as the functor that assigns to a scheme S the isomorphism classes of $(\underline{a}, \delta)$-(semi)stable ϱ-flagged pseudo G-bundles parameterized by S. In order to obtain the moduli spaces, we proceed as follows.
The natural transformation from the functor of isomorphism classes of families of ϱ-flagged pseudo G-bundles into the functor of decorated flagged vector bundles gives rise to the $\mathrm{GL}(Y)$-equivariant morphism

$$\begin{array}{ccc} \mathrm{AD}\colon \mathfrak{F}_{\varrho\text{-FLPsBun}} & \longrightarrow & \mathfrak{P}\,. \\ & \searrow \quad \swarrow & \\ & \mathfrak{Q} & \end{array}$$

The subgroup $\mathbb{G}_m(k) = \mathbb{G}_m(k) \cdot \mathrm{id}_V$ acts trivially on $\mathfrak{P}$ and $\mathfrak{Q}$, so that AD induces the $\mathrm{SL}(Y)$-equivariant morphism

$$\begin{array}{ccc} \overline{\mathrm{AD}}\colon \mathfrak{F}_{\varrho\text{-FLPsBun}}/\!\!/\mathbb{G}_m(k) & \longrightarrow & \mathfrak{P}\,. \\ & \searrow \quad \swarrow & \\ & \mathfrak{Q} & \end{array}$$

By Proposition 5.3.1, the scheme $\mathfrak{F}_{\varrho\text{-FLPsBun}}/\!\!/\mathbb{G}_m(k)$ is proper over $\mathfrak{Q}$, so that $\overline{\mathrm{AD}}$ is a proper morphism. According to Lemma 5.1.8, it is also an injective map. Altogether, we realize that $\overline{\mathrm{AD}}$ is a finite map.

Theorem 5.2.2 claims that there are the $\mathrm{SL}(Y)$-invariant open subsets $\mathfrak{P}^{(\underline{a},\delta)\text{-(s)s}}$ that correspond to the $(\underline{a},\delta)$-(semi)stable decorated flagged vector bundles. By definition,

$$\mathfrak{F}^{(\underline{a},\delta)\text{-(s)s}}_{\varrho\text{-FLPsBun}} := \mathrm{AD}^{-1}\big(\mathfrak{P}^{(\underline{a},\delta)\text{-(s)s}}\big)$$

is set the of $(\underline{a},\delta)$-(semi)stable ϱ-flagged pseudo G-bundles, and we find

$$\mathfrak{F}^{(\underline{a},\delta)\text{-(s)s}}_{\varrho\text{-FLPsBun}} /\!\!/ \mathbb{G}_m(k) = \overline{\mathrm{AD}}^{-1}\big(\mathfrak{P}^{(\underline{a},\delta)\text{-(s)s}}\big).$$

We have seen that the good quotient $\mathfrak{P}^{(\underline{a},\delta)\text{-ss}} /\!\!/ \mathrm{SL}(Y)$ exists as a projective scheme that contains the geometric quotient $\mathfrak{P}^{(\underline{a},\delta)\text{-s}} / \mathrm{SL}(Y)$ as an open subscheme. Since $\overline{\mathrm{AD}}$ is finite, the quotients

$$\mathscr{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-(s)s}} := \big(\mathfrak{F}^{(\underline{a},\delta)\text{-(s)s}}_{\varrho\text{-FLPsBun}} /\!\!/ \mathbb{G}_m(k)\big) /\!\!/ \mathrm{SL}(Y)$$

also exist. The scheme $\mathscr{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-ss}}$ is a projective good quotient and $\mathscr{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-s}}$, an open subscheme of $\mathscr{M}^{(\underline{a},\delta)\text{-ss}}(\varrho,\underline{r})$, is a geometric quotient. Since

$$\begin{aligned}\big(\mathfrak{F}^{(\underline{a},\delta)\text{-(s)s}}_{\varrho\text{-FLPsBun}} /\!\!/ \mathbb{G}_m(k)\big) /\!\!/ \mathrm{SL}(Y) &= \mathfrak{F}^{(\underline{a},\delta)\text{-(s)s}}_{\varrho\text{-FLPsBun}} /\!\!/ \big(\mathbb{G}_m(k)\times \mathrm{SL}(Y)\big)\\ &= \mathfrak{F}^{(\underline{a},\delta)\text{-(s)s}}_{\varrho\text{-FLPsBun}} /\!\!/ \mathrm{GL}(Y),\end{aligned}$$

the scheme $\mathscr{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-ss}}$ is the moduli space we were striving at. (More details on the above arguments may be found in the paper [15].) This construction implies the following result.

Theorem 5.3.2. *The coarse moduli spaces* $\mathscr{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-(s)s}}$ *for the functors* $\mathrm{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-(s)s}}$ *exist, the scheme* $\mathscr{M}(\varrho,\underline{x},\underline{r})^{(\underline{a},\delta)\text{-ss}}$ *being projective.*

Remark 5.3.3. The construction of this moduli space does not immediately generalize to curves over a base ring. Let us explain the remedy.
We assume that G and the representation $\varrho\colon G \longrightarrow \mathrm{GL}(V_{\mathbb{Z}})$ are defined over the integers. By Seshadri's generalization of GIT relative to base varieties which are defined over Nagata rings [39], the algebra

$$\mathrm{Sym}^\star(V_{\mathbb{Z}}\otimes \mathbb{Z}^r)^G$$

is a finitely generated $\mathbb{Z}$-algebra, and we have the good quotients

$$\pi\colon \mathrm{Hom}(V_{\mathbb{Z}},\mathbb{Z}^r) \longrightarrow \mathrm{Hom}(V_{\mathbb{Z}},\mathbb{Z}^r)/\!\!/G := \mathrm{Spec}\big(\mathrm{Sym}^\star(V_{\mathbb{Z}}\otimes\mathbb{Z}^r)^G\big) \longrightarrow \mathrm{Spec}(\mathbb{Z})$$

and

$$\overline{\pi}\colon \mathbb{P}\big(\mathrm{Hom}(V_{\mathbb{Z}},\mathbb{Z}^r)^\vee\big) \dashrightarrow \mathbb{P}\big(\mathrm{Hom}(V_{\mathbb{Z}},\mathbb{Z}^r)^\vee\big)/\!\!/G := \mathrm{Proj}\big(\mathrm{Sym}^\star(V_{\mathbb{Z}}\otimes\mathbb{Z}^r)^G\big) \longrightarrow \mathrm{Spec}(\mathbb{Z}).$$

The quotient

$$\pi^0\colon \mathrm{Isom}(V_{\mathbb{Z}}, \mathbb{Z}^r) \longrightarrow \mathrm{Isom}(V_{\mathbb{Z}}, \mathbb{Z}^r)/G$$

is a principal G-bundle and thus a universal categorical quotient. However, the quotients π and $\overline{\pi}$ are not necessarily universal categorical quotients. This fact accounts for the slight modifications which we do have to make. The good quotient parameterizes orbits of geometric points with respect to the equivalence relation that two points map to the same point in the quotient, if and only if the closures of their orbits intersect. This implies the following.

Lemma 5.3.4. *Let $Z \hookrightarrow \mathrm{Spec}(\mathbb{Z})$ be a closed subscheme. Then, the canonical morphisms*

$$\big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r) \times_{\mathrm{Spec}(\mathbb{Z})} Z\big)/\!\!/G \longrightarrow \big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)/\!\!/G\big) \times_{\mathrm{Spec}(\mathbb{Z})} Z$$

and

$$\Big(\mathbb{P}\big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)^\vee\big) \times_{\mathrm{Spec}(\mathbb{Z})} Z\Big)/\!\!/G \longrightarrow \Big(\mathbb{P}\big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)^\vee\big)/\!\!/G\Big) \times_{\mathrm{Spec}(\mathbb{Z})} Z$$

are bijective on geometric points.

Let us write

$$\big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r) \times_{\mathrm{Spec}(\mathbb{Z})} Z\big)\widetilde{/\!\!/}G := \big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)/\!\!/G\big) \times_{\mathrm{Spec}(\mathbb{Z})} Z$$

and

$$\Big(\mathbb{P}\big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)^\vee\big) \times_{\mathrm{Spec}(\mathbb{Z})} Z\Big)\widetilde{/\!\!/}G := \Big(\mathbb{P}\big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)^\vee)\big)/\!\!/G\Big) \times_{\mathrm{Spec}(\mathbb{Z})} Z.$$

Next, assume that E is a locally free sheaf on the scheme Y which is of finite type over $\mathrm{Spec}(R)$, R a Nagata ring. Then, we may easily construct the geometric quotient

$$\begin{aligned}&\widetilde{\mathscr{H}} := \mathscr{H}\!om(V \otimes \mathscr{O}_Y, E)\widetilde{/\!\!/}G :=\\ &\Big(\mathscr{I}\!som(R^r \otimes \mathscr{O}_Y, E) \times_{\mathrm{Spec}(R)} \big(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r) \times_{\mathrm{Spec}(\mathbb{Z})} \mathrm{Spec}(R)\big)\widetilde{/\!\!/}G\Big)/\mathrm{GL}_r(R),\end{aligned}$$

using local trivializations. The construction of $\mathscr{H}\!om(V \otimes \mathscr{O}_Y, E)\widetilde{/\!\!/}G$ clearly commutes with base changes $Y' \longrightarrow Y$. Moreover, we have the natural morphism

$$\mathscr{H}\!om(V \otimes \mathscr{O}_Y, E)/\!\!/G \longrightarrow \mathscr{H}\!om(V \otimes \mathscr{O}_Y, E)\widetilde{/\!\!/}G$$

which is bijective, by Lemma 5.3.4. This construction has an algebraic counterpart. Define $\widetilde{\pi}\colon \widetilde{\mathscr{H}} \longrightarrow Y$ as the projection map, and let

$$\widetilde{\mathscr{S}\!ym}^\star(E^\vee \otimes V)^G$$

be the sheaf $\widetilde{\pi}_\star(\mathscr{O}_{\widetilde{\mathscr{H}}})$. Then, we obtain the homomorphism

$$\mathrm{ps}(E)\colon \widetilde{\mathscr{S}\!ym}^\star(E^\vee \otimes V)^G \longrightarrow \mathscr{S}\!ym^\star(E^\vee \otimes V)^G$$

that induces the bijective map $\mathscr{H}om(V \otimes \mathscr{O}_Y, E)/\!\!/G \longrightarrow \widetilde{\mathscr{H}}$.

Now, assume that $\mathscr{C} \longrightarrow \mathrm{Spec}(R)$ is a curve over the Nagata ring R and that $S \longrightarrow \mathrm{Spec}(R)$ is a scheme of finite type over R. Then, a *family of weak pseudo G-bundles on $\mathscr{C}$ parameterized by S*, is a pair $(E_S, \widetilde{\tau_S})$ that consists of a locally free sheaf E_S of rank $\dim(V)$ on $S \times_{\mathrm{Spec}(R)} \mathscr{C}$, such that $\det(E_S)$ is a pullback from S, and a homomorphism

$$\widetilde{\tau}\colon \widetilde{\mathscr{S}ym}^\star(E_S^\vee \otimes V)^G \longrightarrow \mathscr{O}_{S \times_{\mathrm{Spec}(R)} \mathscr{C}}$$

whose fibers over S are non-trivial. Unlike the pseudo G-bundles that we had considered before, there is a pull-back for weak pseudo G-bundles, so that there are reasonable stacks and moduli functors for them. In the same manner, we can define *ϱ-flagged weak pseudo G-bundles* and families of such.

Next, suppose that the algebra $\mathrm{Sym}^\star(V_{\mathbb{Z}} \otimes \mathbb{Z}^r)^G$ is generated in degrees $\le s$. By Remark 5.1.6, we may write

$$\bigoplus_{\substack{(d_1,\dots,d_s):\\ d_i \ge 0,\ \sum i d_i = s!}} \mathrm{Sym}^{d_1}\big((V_{\mathbb{Z}} \otimes \mathbb{Z}^r)^G\big) \otimes \cdots \otimes \mathrm{Sym}^{d_s}\big(\mathrm{Sym}^i(V_{\mathbb{Z}} \otimes \mathbb{Z}^r)^G\big)$$

as the quotient of $\mathbb{D}^{s!,v}(\mathbb{Z}^r)$, for an appropriate integer $v > 0$. As before, we may therefore associate with a family of ϱ-flagged weak pseudo G-bundles a family of ϱ-flagged decorated vector bundles.

We also point out the following result:

Lemma 5.3.5. *Let G be a reductive algebraic group, X and Y projective schemes equipped with a G-action, and $\pi\colon X \longrightarrow Y$ a finite and G-equivariant morphism. Suppose $\mathscr{L}$ is a G-linearized ample line bundle on Y. Then, for any point $x \in X$ and any one-parameter subgroup $\lambda\colon \mathbb{G}_m \longrightarrow G$, one has*

$$\mu_{\pi^\star(\mathscr{L})}(\lambda, x) = \mu_{\mathscr{L}}\big(\lambda, \pi(x)\big).$$

Proof. This is Lemma 2.1 in [38] and also holds in positive characteristic: simply replace the G-module splitting by a splitting of the induced $\mathbb{G}_m$-module. □

In particular, we may apply this lemma to the finite morphism

$$\pi\colon \mathbb{P}\big(\mathrm{Hom}(V, k^r)^\vee\big)/\!\!/G \longrightarrow \mathbb{P}\big(\mathrm{Hom}(V, k^r)^\vee\big)\widetilde{/\!\!/}G.$$

(Note that the ample line bundle $\mathscr{N}$ on the left hand space with which we compute the μ-function is indeed the pullback of the ample line bundle $\mathscr{L}$ on the right hand space with respect to which we compute the μ-function. Indeed, for $r \gg 0$, $\mathscr{N}$ is constructed from the invariant global sections in $\mathscr{O}_{\mathbb{P}(\mathrm{Hom}(V,k^r)^\vee)}(r)$ whereas $\mathscr{L}$ is constructed from those invariant sections that extend to $\mathbb{P}(\mathrm{Hom}(V_{\mathbb{Z}}, \mathbb{Z}^r)^\vee)$.) The lemma therefore shows that, if we use the above new construction to associate with a principal G-bundle $\mathscr{P} = (E, \tau)$ a decorated vector bundle (E, φ), we may still characterize those weighted

filtrations $(E_\bullet, \beta_\bullet)$ that arise from reductions of $\mathscr{P}$ to one-parameter subgroups of G by the condition "$\mu(E_\bullet, \beta_\bullet; \varphi) = 0$", as in [15], Lemma 5.4.2.
These considerations clearly show that the moduli spaces of ϱ-flagged weak pseudo G-bundles on $\mathscr{C}$ may be constructed from the moduli spaces of ϱ-flagged decorated vector bundles in the same way as before.
Note that, for ϱ-flagged principal G-bundles, nothing changes, because $\mathscr{I}som(V \otimes \mathscr{O}_Y, E)/G$ is still an open subscheme of $\mathscr{H}om(V \otimes \mathscr{O}_Y, E)\widetilde{/\!\!/}G$.

S-equivalence. — As usual, the points in the moduli space will be in one to one correspondence to the S-equivalence classes of $(\underline{a}, \delta)$-semistable pseudo G-bundles. So, in order to identify the closed points of $\mathscr{M}(\varrho, \underline{x}, \underline{r})^{(\underline{a},\delta)\text{-ss}}$, we have to explain this equivalence relation.
Suppose that $(E, \tau, \underline{q})$ is an $(\underline{a}, \delta)$-semistable ϱ-flagged pseudo G-bundle with associated decorated flagged vector bundle $(E, \underline{q}, \varphi)$ and that $(E_\bullet, \beta_\bullet)$ is a weighted filtration of E with

$$M_{\underline{a}}(E_\bullet, \beta_\bullet) + \delta \cdot \mu\bigl(E_\bullet, \beta_\bullet; \varphi\bigr) = 0.$$

We first define the *associated admissible deformation* $\mathrm{df}_{(E_\bullet,\beta_\bullet)}(E, \tau, \underline{q}) = (E_{\mathrm{df}}, \tau_{\mathrm{df}}, \underline{q}_{\mathrm{df}})$. We set $E_{\mathrm{df}} = \bigoplus_{i=0}^{t} E_{i+1}/E_i$. Let $\lambda\colon \mathbb{G}_m(k) \longrightarrow \mathrm{SL}_r(k)$ be a one-parameter subgroup whose weighted flag $(W_\bullet(\lambda), \beta_\bullet(\lambda))$ in k^r satisfies:

- $\dim(W_i) = \mathrm{rk}(E_i)$, $i = 1, ..., t$, in $W_\bullet(\lambda) : 0 \subsetneq W_1 \subsetneq \cdots \subsetneq W_t \subsetneq k^r$;
- $\beta_\bullet(\lambda) = \beta_\bullet$.

Then, the given filtration $E_\bullet$ corresponds to a reduction of the structure group of $\mathscr{I}som(\mathscr{O}_C^{\oplus r}, E)$ to $Q(\lambda)$. On the other hand, λ defines a decomposition

$$\mathrm{Sym}^\star\bigl(V \otimes (k^r)^\vee\bigr)^G = \bigoplus_{i\in\mathbb{Z}} U^i,$$

U^i being the eigenspace to the character $z \longmapsto z^i$, $i \in \mathbb{Z}$. With $U_i := \bigoplus_{j\le i} U^i$, we define the filtration

$$\cdots \subset U_{i-1} \subset U_i \subset U_{i+1} \subset \cdots \subset \mathrm{Sym}^\star\bigl(V \otimes (k^r)^\vee\bigr)^G. \tag{7}$$

Observe that $Q(\lambda)$ fixes this filtration. Thus, we obtain a $Q(\lambda)$-module structure on

$$\bigoplus_{i\in\mathbb{Z}} U_i/U_{i-1} \cong \mathrm{Sym}^\star\bigl(V \otimes (k^r)^\vee\bigr)^G. \tag{8}$$

Next, we write $Q(\lambda) = \mathscr{R}_u(Q(\lambda)) \rtimes L(\lambda)$ where $L(\lambda) \cong \mathrm{GL}(W_1/W_0) \times \cdots \times \mathrm{GL}(k^r/W_t)$ is the centralizer of λ. Note that (8) is an isomorphism of $L(\lambda)$-modules. The process of passing from E to E_{df} corresponds to first reducing the structure group to $Q(\lambda)$, then extending it to $L(\lambda)$ via

$Q(\lambda) \longrightarrow Q(\lambda)/\mathscr{R}_u(Q(\lambda)) \cong L(\lambda)$, and then extending it to $\mathrm{GL}_r(k)$ via the inclusion $L(\lambda) \subset \mathrm{GL}_r(k)$. By (7), there is a filtration

$$\cdots \subset \mathscr{U}_{i-1} \subset \mathscr{U}_i \subset \mathscr{U}_{i+1} \subset \cdots \subset \mathscr{S}ym^\star(V \otimes E^\vee)^G,$$

and, by (8), we have a canonical isomorphism

$$\mathscr{S}ym^\star(V \otimes E_{\mathrm{df}}^\vee)^G \cong \bigoplus_{i \in \mathbb{Z}} \mathscr{U}_i/\mathscr{U}_{i-1}. \tag{9}$$

Observe that the modules $\mathscr{U}_i$ and $\mathscr{U}_i/\mathscr{U}_{i-1}$, $i \in \mathbb{Z}$, are graded by the degree in the algebra $\mathscr{S}ym^\star(V \otimes E^\vee)^G$, so that the algebra in (9) is in fact bigraded. We now look at the subalgebra $\mathscr{S}_\mu$ consisting of the components of bidegree (d,i) where either $d=0$ or $d>0$ and

$$\frac{i}{d} = \frac{1}{s!} \cdot \mu(E_\bullet, \beta_\bullet; \varphi).$$

Then, τ clearly induces a non-trivial homomorphism τ_μ on $\mathscr{S}_\mu$, and we define τ_{df} as τ_μ on $\mathscr{S}_\mu$ and as zero on the other components. The flagging $\underline{q}_{\mathrm{df}}$ of E_{df} is obtained by a similar procedure.

Remark 5.3.6. If $(E,\tau,\underline{q})$ is a ϱ-flagged *principal* G-bundle and $\delta \gg 0$, the arguments of [15], proof of Theorem 5.4.1, show that admissible deformations are associated with weighted filtrations $(E_\bullet, \beta_\bullet)$, such that $M_{\underline{a}}(E_\bullet,\beta_\bullet) = 0$ and $\mu(E_\bullet,\beta_\bullet;\varphi) = 0$. In that case, $\mathscr{S}_0 = \mathscr{U}_0$. Recall that $\mu(E_\bullet,\beta_\bullet;\varphi) = 0$ means that $(E_\bullet,\beta_\bullet)$ comes from a reduction of $\mathscr{P} = (E,\tau)$ to a parabolic subgroup ([15], Lemma 5.4.2).

A ϱ-flagged pseudo G-bundle $(E,\tau,\underline{q})$ is said to be $(\underline{a},\delta)$-*polystable*, if it is $(\underline{a},\delta)$-semistable and equivalent to every admissible deformation $\mathrm{df}_{(E_\bullet,\beta_\bullet)}(E,\tau,\underline{q}) = (E_{\mathrm{df}},\tau_{\mathrm{df}},\underline{q}_{\mathrm{df}})$ associated with a filtration $(E_\bullet,\beta_\bullet)$ of E with $M_{\underline{a}}(E_\bullet,\beta_\bullet) + \delta \cdot \mu\bigl(E_\bullet,\beta_\bullet;\varphi\bigr) = 0$.

Lemma 5.3.7. *Let $(E,\tau,\underline{q})$ be an $(\underline{a},\delta)$-semistable ϱ-flagged pseudo G-bundle. Then, there exists an $(\underline{a},\delta)$-polystable admissible deformation* $\mathrm{gr}(E,\tau,\underline{q})$ *of $(E,\tau,\underline{q})$. The ϱ-flagged pseudo G-bundle* $\mathrm{gr}(E,\tau,\underline{q})$ *is unique up to equivalence.*

In general, not every admissible deformation will immediately lead to a polystable ϱ-flagged pseudo G-bundle, but any iteration of admissible deformations (leading to non-equivalent ϱ-flagged pseudo G-bundles) will do so after finitely many steps. We call two $(\underline{a},\delta)$-semistable ϱ-flagged pseudo G-bundles $(E,\tau,\underline{q})$ and $(E',\tau',\underline{q}')$ *S-equivalent*, if $\mathrm{gr}(E,\tau,\underline{q})$ and $\mathrm{gr}(E',\tau',\underline{q}')$ are equivalent.

Sketch of proof of Lemma 5.3.7. The lemma follows from our GIT construction of the moduli space. As is well-known, two points $y,y' \in \mathfrak{F}^{(\underline{a},\delta)\text{-ss}}$, $\mathfrak{F} := \mathfrak{F}_{\varrho\text{-FLPsBun}}$, will be mapped to the same point in the quotient, if and only if the closures of their orbits intersect. Let us call the resulting equivalence relation *orbit equivalence*. Let $y \in \mathfrak{F}^{(\underline{a},\delta)\text{-ss}}$ be a point and $\lambda\colon \mathbb{G}_m(k) \longrightarrow \mathrm{SL}(Y)$ a one parameter subgroup with $\mu(\lambda, y) = 0$. Define $y_\infty(\lambda) := \lim_{z\to\infty} \lambda(z)\cdot y$. By the Hilbert–Mumford criterion (see [32], p. 53, i), and Lemma 0.3), orbit equivalence is the equivalence relation that is generated by $y \sim y_\infty(\lambda)$, $y \in \mathfrak{F}^{(\underline{a},\delta)\text{-ss}}$, λ a one-parameter subgroup of $\mathrm{SL}(Y)$ with $\mu(\lambda, y) = 0$.

On the other hand, if y represents the ϱ-flagged pseudo G-bundle $(E, \tau, \underline{q})$, then λ induces a weighted filtration $(E_\bullet, \beta_\bullet)$ with $M_{\underline{a}}(E_\bullet, \beta_\bullet) + \delta \cdot \mu(E_\bullet, \beta_\bullet; \varphi) = 0$ and $y_\infty(\lambda)$ represents the admissible deformation $\mathrm{df}_{(E_\bullet,\beta_\bullet)}(E, \tau, \underline{q})$. Conversely, any admissible deformation of $(E, \tau, \underline{q})$ comes from a one-parameter subgroup λ of $\mathrm{SL}(Y)$ with $\mu(\lambda, y) = 0$. The assertion of the lemma now results from the fact that the closure of any orbit contains a unique closed orbit.

The details of the above proof consist of a very careful but routine analysis of the computations with the Hilbert–Mumford criterion (which will be performed in Section 5.6). □

Corollary 5.3.8. *The closed points of the moduli space $\mathscr{M}(\varrho, \underline{x}, \underline{r})^{(\underline{a},\delta)\text{-ss}}$ are in one to one correspondence to the S-equivalence classes of $(\underline{a}, \delta)$-semistable ϱ-flagged pseudo G-bundles of type $\underline{r}$, or, equivalently, to the isomorphism classes of $(\underline{a}, \delta)$-polystable ϱ-flagged pseudo G-bundles of type $\underline{r}$.*

5.4 The Moduli Spaces for ϱ-Flagged Principal G-Bundles

Let us remind the reader of the set-up for ϱ-flagged principal G-bundles. First, we fix an element $\vartheta \in \pi_1(G)$, a tuple $\underline{x} = (x_1, ..., x_b)$ of distinct k-rational points on C, and a tuple $\underline{P} = (P_1, ..., P_b)$ of parabolic subgroups of $\mathrm{GL}(V)$. The tuple $\underline{P}$ gives rise to a tuple $\underline{r} = (r_{ij}, j = 1, ..., t_i, i = 1, ..., b)$ of positive integers.

Let $\underline{a} = (a_1, ..., a_b)$ be a stability parameter where $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$, $i = 1, ..., b$. Then, representing a_i by a rational one-parameter subgroup, we obtain a weighted flag $(V_\bullet(a_i), \beta_\bullet(a_i))$ in V, $i = 1, ..., b$. The tuple $\beta_\bullet(a_i)$ does not depend on the choice of the representative for a_i. Hence, we get the well-defined tuple $\underline{a}^\varrho = (a^\varrho_{ij}, j = 1, ..., t_i, i = 1, ..., b)$ via

$$\left(a^\varrho_{i1}, ..., a^\varrho_{it_i}\right) := r \cdot \beta_\bullet(a_i), \quad i = 1, ..., b.$$

Proposition 5.4.1. *There is a positive rational number δ_0, such that for every rational number $\delta > \delta_0$ and every ϱ-flagged principal G-bundle $(\mathscr{P}, \underline{s})$ of type $(\underline{x}, \underline{P})$ with associated ϱ-flagged pseudo G-bundle $(E, \tau, \underline{q})$ of type $(\underline{x}, \underline{r})$ the following properties are equivalent:*

i) *$(\mathscr{P}, \underline{s})$ is an $\underline{a}$-(semi)stable ϱ-flagged principal G-bundle.*

ii) *$(E, \tau, \underline{q})$ is an $(\underline{a}^\varrho, \delta)$-(semi)stable ϱ-flagged pseudo G-bundle.*

Proof. First note that the set of isomorphism classes of $\underline{a}$-semistable ϱ-flagged principal G-bundles of type $(\underline{x}, \underline{P})$ is bounded. Indeed, given a parabolic subgroup Q of G, we write the pair $(Q, \det_Q)$ as $(Q_G(\lambda), \chi_{-\lambda})$ for some one-parameter subgroup λ of G. Since there only finitely many conjugacy classes of parabolic subgroups of G, it is clear that we may find a constant D_1 with

$$\big\langle (\widetilde{\chi}_\lambda)_{s_i}, a_{s_i} \big\rangle = -\big\langle (\widetilde{\chi}_{-\lambda})_{s_i}, a_{s_i} \big\rangle \geq D_1,$$

for any reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to Q and $i = 1, ..., b$. The condition of $\underline{a}$-semistability thus gives the estimate

$$\deg\big(\mathscr{P}_Q(\det_Q)\big) \geq \sum_{i=1}^{b} \big\langle (\widetilde{\chi}_\lambda)_{s_i}, a_{s_i} \big\rangle \geq b \cdot D_1.$$

Therefore, the degree of instability of $\mathscr{P}$ as a principal G-bundle is bounded from below by a constant that depends only on the input data. As is well known (see, e.g., [4]) this implies that $\mathscr{P}$ belongs to a bounded family of isomorphism classes of principal G-bundles.
Using Proposition 5.1.3, the rest of the arguments are now identical to those given in the proof of Theorem 5.4.1 in [15]. □

As is obvious from Lemma 5.1.4, there is an open and $\mathrm{GL}(Y)$-invariant subscheme

$$\mathfrak{F}_{\varrho\text{-FlBun}} \subset \mathfrak{F}_{\varrho\text{-FlPsBun}}$$

that parameterizes the ϱ-flagged principal G-bundles. We claim that

$$\mathfrak{F}^{\underline{a}\text{-ss}}_{\varrho\text{-FlBun}} := \mathfrak{F}^{(\underline{a}^\varrho, \delta)\text{-ss}}_{\varrho\text{-FlPsBun}} \cap \mathfrak{F}_{\varrho\text{-FlBun}}$$

is a saturated open subset, i.e., for every point $f \in \mathfrak{F}^{\underline{a}\text{-ss}}_{\varrho\text{-FlBun}}$, the closure of the orbit $\mathrm{GL}(Y) \cdot f$ inside $\mathfrak{F}^{(\underline{a}^\varrho, \delta)\text{-ss}}_{\varrho\text{-FlPsBun}}$ is contained in $\mathfrak{F}^{\underline{a}\text{-ss}}_{\varrho\text{-FlBun}}$. The discussion of S-equivalence of ϱ-flagged pseudo G-bundles shows that this statement is equivalent to the fact that the set of isomorphism classes of $\underline{a}$-semistable ϱ-flagged principal bundles is closed under S-equivalence inside the set of isomorphism classes of $(\underline{a}^\varrho, \delta)$-semistable ϱ-flagged pseudo G-bundles. To see this, note that, by Remark 5.3.6, an admissible deformation of the ϱ-flagged principal bundle $(E, \tau, \underline{q})$ is associated with a weighted filtration $(E_\bullet(\mathscr{P}_Q), \beta_\bullet(\mathscr{P}_Q))$, coming from a reduction $\mathscr{P}_Q$ of $\mathscr{P}$ to a parabolic subgroup Q of G, such that

$$M_{\underline{a}}\big(E_\bullet(\mathscr{P}_Q), \beta_\bullet(\mathscr{P}_Q)\big) = 0.$$

It is easy to verify that $(E_{\mathrm{df}}, \tau_{\mathrm{df}})$ in $\mathrm{df}_{(E_\bullet(\delta), \beta_\bullet(\delta))}(E, \tau, \underline{q}) = (E_{\mathrm{df}}, \tau_{\mathrm{df}}, \underline{q}_{\mathrm{df}})$ defines again a principal G-bundle. (In fact, $\mathscr{P}$ is obtained from $\mathscr{P}_Q$ by means of extending the structure group via $Q \subset G$. Extending the structure group of $\mathscr{P}_Q$ via $Q \longrightarrow L \subset G$, L a Levi subgroup of Q, yields the principal bundle $\mathscr{P}_{\mathrm{df}}$ corresponding to $(E_{\mathrm{df}}, \tau_{\mathrm{df}})$.)

Since $\mathfrak{F}^{\underline{a}\text{-ss}}_{\varrho\text{-FlBun}}$ is a saturated subset of $\mathfrak{F}^{(\underline{a}^\varrho,\delta)\text{-ss}}_{\varrho\text{-FlPsBun}}$, there is an open subset $U \subset \mathfrak{F}^{(\underline{a}^\varrho,\delta)\text{-ss}}_{\varrho\text{-FlPsBun}}/\!\!/ \operatorname{GL}(Y)$, such that $\mathfrak{F}^{\underline{a}\text{-ss}}_{\varrho\text{-FlBun}}$ is the preimage of U under the quotient map $\mathfrak{F}^{(\underline{a}^\varrho,\delta)\text{-ss}}_{\varrho\text{-FlPsBun}} \longrightarrow \mathfrak{F}^{(\underline{a}^\varrho,\delta)\text{-ss}}_{\varrho\text{-FlPsBun}}/\!\!/ \operatorname{GL}(Y)$, and

$$U = \mathfrak{F}^{\underline{a}\text{-ss}}_{\varrho\text{-FlBun}}/\!\!/ \operatorname{GL}(Y)$$

is the good quotient. Likewise, we see that the geometric quotient $\mathfrak{F}^{\underline{a}\text{-s}}_{\varrho\text{-FlBun}}/ \operatorname{GL}(Y)$ does exist. We define

$$\mathscr{M}(\vartheta,\varrho,\underline{x},\underline{P})^{\underline{a}\text{-(s)s}} := \mathfrak{F}^{\underline{a}\text{-(s)s}}_{\varrho\text{-FlBun}}/\!\!/ \operatorname{GL}(Y).$$

Theorem 5.4.2. *Assume that the stability parameter $\underline{a}$ is such that $\sum_{j=1}^{t_i} a^\varrho_{ij} < 1$ for $i = 1,...,b$. Then, the moduli spaces $\mathscr{M}(\vartheta,\varrho,\underline{x},\underline{P})^{\underline{a}\text{-(s)s}}$ for the functors that assign to a scheme S the set of isomorphism classes of families of $\underline{a}$-(semi)stable ϱ-flagged principal G-bundles of topological type ϑ and type $(\underline{x},\underline{P})$ exist as quasi-projective schemes.*

Finally, we note that the same argument as in Theorem 5.4.4 in [15] gives the following result:

Theorem 5.4.3 (Semistable reduction). *Assume that the representation $\varrho\colon G \longrightarrow \operatorname{GL}(V)$ is of low separable index or that G is an adjoint group, $\varrho\colon G \longrightarrow \operatorname{GL}(\operatorname{Lie}(G))$ is the adjoint representation, and that the characteristic of k is larger than the height of ϱ. Then, $\mathscr{M}(\vartheta,\varrho,\underline{x},\underline{P})^{\underline{a}\text{-(s)s}}$ is projective.*

5.5 The Moduli Spaces for Flagged Principal G-Bundles

We fix $\vartheta \in \pi_1(G)$, $\underline{x} = (x_1,...,x_b)$, and the tuple $\underline{P} = (P_1,...,P_s)$ of parabolic subgroups of G. Let $\underline{a} = (a_1,...,a_b)$ be a stability parameter with $a_i \in X^\star(P_i)^\vee_{\mathbb{Q},+}$, $i = 1,...,b$.
For the moment, let $\varrho\colon G \longrightarrow \operatorname{GL}(V)$ be any (not necessarily faithful) representation. We assume that we may represent the a_i by rational one-parameter subgroups that do not lie in the kernel of ϱ. Then, the same construction as in the last section provides us with a tuple $\underline{a}^\varrho = (a^\varrho_{ij}, j = 1,...,t_i, i = 1,...,b)$ of positive rational numbers. We say that the stability parameter $\underline{a}$ is *ϱ-admissible*, if the condition

$$\sum_{j=1}^{t_i} a^\varrho_{ij} < 1, \quad i = 1,...,b,$$

is verified.

Lemma 5.5.1. *The stability parameter $\underline{a}$ is* Ad*-admissible, if and only it is admissible in the sense of the definition following Remark* 4.1.5.

Proof. Let a be a rational one-parameter subgroup of the maximal torus $T \subset G$. The eigenspaces of a are direct sums of root spaces, and a acts on the space for the root α with the weight $\langle\alpha, a\rangle$. The Lie algebra of T is contained in the eigenspace to the weight zero. Since, for every root α, $-\alpha$ is also a root, the weights of the eigenspaces of a are (in increasing order) $-\gamma_s, ..., -\gamma_1, 0, \gamma_1, ..., \gamma_s$. If $(a_1, ..., a_t) = \dim(G) \cdot \beta_\bullet(a)$, we infer

$$\sum_{j=1}^{t} a_j = 2\gamma_s.$$

The condition $\sum_{j=1}^{t} a_j < 1$ thus amounts to the condition $\gamma_s < 1/2$. Since $|\langle\alpha, a\rangle| \leq \gamma_s$ for all roots and equality holds for at least one root, these considerations establish our claim. □

Note that there is a $\mathrm{GL}(Y)$-invariant closed subscheme

$$\mathfrak{F}_{\mathrm{FlBun}} \hookrightarrow \mathfrak{F}_{\varrho\text{-FlBun}}$$

that parameterizes the flagged principal G-bundles. Recall that we have verified in Lemma 5.1.2 the compatibility of the notions of (semi)stability. Theorem 5.4.2 thus immediatly implies:

Theorem 5.5.2. *Let $\underline{a}$ be a stability parameter, such that there exists a faithful representation $\varrho\colon G \longrightarrow \mathrm{GL}(V)$ for which $\underline{a}$ is ϱ-admissible. Then, the moduli spaces $\mathscr{M}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-(s)s}}$ for the functors of isomorphism classes of families of $\underline{a}$-(semi)stable flagged principal G-bundles of topological type ϑ and type $(\underline{x}, \underline{P})$ exist as quasi-projective schemes. They are projective by Theorem* 4.4.1.

Corollary 5.5.3. *Assume that the stability parameter $\underline{a}$ is admissible. Then, the moduli spaces $\mathscr{M}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-(s)s}}$ exist as projective schemes.*

Proof. If G is an adjoint group, the quasi-projectivity of the moduli space is a restatement of Theorem 5.4.2, taking into account Lemma 5.5.1. Properness follows from Theorem 4.4.1.
In general, one can use Ramanathan's method to construct the moduli space for an arbitrary semisimple group from the one of the adjoint group. (Observe that every flagged principal G-bundle $(\mathscr{P}, \underline{s})$ defines in a natural way an adjoint flagged principal G-bundle $\mathrm{Ad}(\mathscr{P}, \underline{s})$, such that $(\mathscr{P}, \underline{s})$ is $\underline{a}$-semistable, if and only if $\mathrm{Ad}(\mathscr{P}, \underline{s})$ is so.) The necessary techniques are described in Section 5 of [16]. □

Remark 5.5.4. i) The corollary gives a complete construction of the moduli spaces of flagged principal G-bundles in all characteristics. Note that we do not need it for our applications, because we are allowed to make the stability parameter $\underline{a}$ as small as we wish to (cf. the proof of Proposition 4.2.2). Thus, having prescribed any faithful representation ϱ, we may for our purposes assume that $\underline{a}$ is ϱ-admissible.
ii) Note that, in our application, we need only the moduli spaces for stability parameters of coprime type. For these stability parameters, the properness of the moduli space implies the semistable reduction theorem, by Lemma 3.3.1.

iii) Suppose that R is, as in Corollary 3.3.4, a ring of finite type over $\mathbb{Z}$, regular and of dimension at most 1. Assume that $\mathscr{C} \longrightarrow \mathrm{Spec}(R)$ is a smooth projective curve. We claim that in this setting, we can construct our moduli space $\mathscr{M}_{\mathscr{C}}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-ss}}$ as a projective scheme over $\mathrm{Spec}(R)$. The only case in which this is not completely obvious is the case when $\mathrm{Spec}(R)$ dominates $\mathrm{Spec}(\mathbb{Z})$. By Remark 5.3.3, we know that we can construct $\mathscr{M}_{\mathscr{C}}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-ss}}$ as a quasi-projective scheme; let $\overline{\mathscr{M}} \longrightarrow \mathrm{Spec}(R)$ be the closure that is obtained as the quotient of the closure of the locus $\underline{a}$-semistable flagged principal G-bundles in $\mathfrak{F}^{(\underline{a},\delta)\text{-ss}}_{\varrho\text{-FLPsBun}}$. By Proposition 2.1.2 and Remark 2.1.3, the moduli space $\mathscr{M}_{\mathscr{C}}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-ss}}$ is irreducible, so that the same holds for $\overline{\mathscr{M}}$. Let C_η be the generic fiber of $\mathscr{C}$ over $\mathrm{Spec}(R)$. We know that the generic fiber of $\overline{\mathscr{M}}$ is the projective moduli space $\mathscr{M}_{C_\eta}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-ss}}$. By the same argument as before, this moduli space is irreducible and, hence, connected. If $r \in \mathrm{Spec}(R)$ is a closed point, and C_r is the fiber of $\mathscr{C}$ over r, then the semistable reduction theorem (Theorem 4.4.1 and 5.4.3) implies that $\mathscr{M}_{C_r}(\vartheta, \underline{x}, \underline{P})^{\underline{a}\text{-ss}}$ is a connected component of the fiber of $\overline{\mathscr{M}}$ over r. Thus, we have to show that $\overline{\mathscr{M}} \longrightarrow \mathrm{Spec}(R)$ has connected fibers. This follows from Stein factorization: indeed, if we factorize $\overline{\mathscr{M}} \longrightarrow \mathrm{Spec}(R') \longrightarrow \mathrm{Spec}(R)$, such that the morphism $\overline{\mathscr{M}} \longrightarrow \mathrm{Spec}(R')$ has connected fibers, then $\mathrm{Spec}(R') \longrightarrow \mathrm{Spec}(R)$ must be an isomorphism. This follows, because it is an isomorphism at the generic point (the generic fiber of $\overline{\mathscr{M}}$ was already connected) and R is assumed to be normal.

5.6 Construction of the Moduli Spaces for Decorated Flagged Vector Bundles

In this section, we will first give the proof of Proposition 5.2.1 by an explicit construction and then carry out the most difficult parts in the proof of Theorem 5.2.2.

Construction of the Parameter Space. — We fix the type $(r, d, \underline{x}, \underline{r}, u, v, L)$. Again, we pick a point $x_0 \in C$ and write $\mathscr{O}_C(1)$ for $\mathscr{O}_C(x_0)$. By Proposition 5.1.10, we can choose an integer n_0, such that, for every $n \geq n_0$ and every $(\underline{a}, \delta)$-semistable decorated flagged vector bundle $(E, \underline{q}, \varphi)$ of type $(r, d, \underline{x}, \underline{r}, u, v, L)$, the following conclusions are true:

- $H^1(E(n)) = \{0\}$ and $E(n)$ is globally generated;
- $H^1(\det(E)(rn)) = \{0\}$ and $\det(E)(rn)$ is globally generated.

Furthermore, we suppose:

- $H^1(L(un)) = \{0\}$ and $L(un)$ is globally generated.

Choose some $n \geq n_0$ and set $l := d + rn + r(1-g)$. Let Y be a k-vector space of dimension l. We define $\mathfrak{Q}^0$ as the quasi-projective scheme parameterizing equivalence classes of quotients $k\colon Y \otimes \mathscr{O}_C(-n) \longrightarrow E$ where E is a vector bundle of rank r and degree d on C and $H^0(k(n))$ is an isomorphism. Then, there is the universal quotient

$$k_{\mathfrak{Q}^0}\colon Y\otimes\pi_C^\star\big(\mathscr{O}_C(-n)\big)\longrightarrow E_{\mathfrak{Q}^0}$$

on $\mathfrak{Q}^0\times C$. Set

$$\mathscr{H}:=\operatorname{Hom}\big(\mathbb{D}^{u,v}(Y),L(un)\big)\quad\text{and}\quad\mathfrak{H}:=\mathbb{P}(\mathscr{H}^\vee)\times\mathfrak{Q}^0.$$

We let

$$k_{\mathfrak{H}}\colon Y\otimes\pi_C^\star\big(\mathscr{O}_C(-n)\big)\longrightarrow E_{\mathfrak{H}}$$

be the pullback of $k_{\mathfrak{Q}^0}$ to $\mathfrak{H}\times C$. Now, on $\mathfrak{H}\times C$, there is the tautological homomorphism

$$s_{\mathfrak{H}}\colon\mathbb{D}^{u,v}(Y)\otimes\mathscr{O}_{\mathfrak{H}}\longrightarrow\pi_C^\star\big(L(un)\big)\otimes\pi_{\mathfrak{H}}^\star\big(\mathscr{O}_{\mathfrak{H}}(1)\big).$$

Let $\mathfrak{T}$ be the closed subscheme defined by the condition that $s_{\mathfrak{H}}\otimes\pi_C^\star(\mathrm{id}_{\mathscr{O}_C(-un)})$ vanishes on

$$\ker\Big(\mathbb{D}^{u,v}(Y)\otimes\pi_C^\star\big(\mathscr{O}_C(-un)\big)\longrightarrow\mathbb{D}^{u,v}(E_{\mathfrak{H}})\Big)\quad\text{(cf. Remark 5.1.7).}$$

Let

$$k_{\mathfrak{T}}\colon Y\otimes\pi_C^\star\big(\mathscr{O}_C(-n)\big)\longrightarrow E_{\mathfrak{T}}$$

be the restriction of $k_{\mathfrak{H}}$ to $\mathfrak{T}\times C$. By definition, there is the universal homomorphism

$$\varphi_{\mathfrak{T}}\colon\mathbb{D}^{u,v}\big(E_{\mathfrak{T}}\big)\longrightarrow\pi_C^\star(L)\otimes\pi_{\mathfrak{T}}^\star(\mathfrak{N}_{\mathfrak{T}}).$$

Here, $\mathfrak{N}_{\mathfrak{T}}$ is the restriction of $\mathscr{O}_{\mathfrak{H}}(1)$ to $\mathfrak{T}$.
Next, let $\mathfrak{G}_{ij}$ be the Graßmann variety that parameterizes the r_{ij}-dimensional quotients of the vector space Y, $j=1,...,t_i$, $i=1,...,s$, and set $\mathfrak{G}:=\times_{j=1,\dots,t_i,i=1,\dots,s}\mathfrak{G}_{ij}$. We construct the parameter space $\mathfrak{P}$ as a closed subscheme of $\mathfrak{T}\times\mathfrak{G}$: on the scheme $\widetilde{\mathfrak{P}}:=\mathfrak{T}\times\mathfrak{G}$, there are the tautological quotients

$$\widetilde{q}_{\widetilde{\mathfrak{P}},ij}\colon Y\otimes\mathscr{O}_{\widetilde{\mathfrak{P}}\times C}\longrightarrow\widetilde{R}_{\widetilde{\mathfrak{P}},ij},\quad j=1,...,t_i,\ i=1,....,s.$$

We define the closed subscheme $\mathfrak{P}$ by the condition that $\widetilde{q}_{\widetilde{\mathfrak{P}},ij}$ vanishes on the kernel of the restriction of $k_{\widetilde{\mathfrak{P}}}$ to $\widetilde{\mathfrak{P}}\times\{x_i\}$, for all $j=1,...,t_i$, $i=1,....,s$. Let $\mathfrak{N}_{\mathfrak{P}}$ be the pullback of $\mathfrak{N}_{\mathfrak{T}}$ to $\mathfrak{P}$. Similarly, we may pull back $k_{\mathfrak{T}}$ and $\varphi_{\mathfrak{T}}$ from $\mathfrak{T}\times C$ to $\mathfrak{P}\times C$ in order to obtain

$$k_{\mathfrak{P}}\colon Y\otimes\pi_C^\star\big(\mathscr{O}_C(-n)\big)\longrightarrow E_{\mathfrak{P}}$$

and

$$\varphi_{\mathfrak{P}}\colon\mathbb{D}^{u,v}\big(E_{\mathfrak{P}}\big)\longrightarrow\pi_C^\star(L)\otimes\pi_{\mathfrak{P}}^\star(\mathfrak{N}_{\mathfrak{P}}).$$

Finally, on $\mathfrak{P} \times \{x_i\}$, we have the quotients

$$q_{\mathfrak{P},ij}\colon E_{\mathfrak{P}|\mathfrak{P}\times\{x_i\}} \longrightarrow R_{\mathfrak{P},ij}, \quad j = 1, ..., t_i,\ i = 1, ..., s.$$

We call $(E_{\mathfrak{P}}; \underline{q}_{\mathfrak{P}}; \varphi_{\mathfrak{P}})$ the *universal family.* This name is justified, because any family of decorated flagged vector bundles parameterized by a scheme S is locally induced by a morphism to $\mathfrak{P}$ and this universal family.
Finally, we note that there is a canonical action of the group $\mathrm{GL}(Y)$ on the parameter space $\mathfrak{P}$, and it will be our task to construct the good and the geometric quotient of the open subsets that parameterize the semistable and the stable objects, respectively. Since the center $\mathbb{G}_m(k) \cdot \mathrm{id}_Y$ acts trivially on $\mathfrak{P}$, it suffices to construct the respective quotients for the action of $\mathrm{SL}(Y)$.

The Map to the Gieseker Space. — Let Jac^d be the Jacobian variety that classifies the line bundles of degree d on C, and choose a Poincaré sheaf $\mathscr{P}$ on $\mathrm{Jac}^d \times C$. By our assumptions on n, the sheaf

$$\mathscr{K}_1 := \mathscr{H}om\Big(\bigwedge^r(Y) \otimes \mathscr{O}_{\mathrm{Jac}^d}, \pi_{\mathrm{Jac}^d\,\star}\big(\mathscr{P} \otimes \pi_C^\star(\mathscr{O}_C(rn))\big)\Big)$$

is locally free. We set $\mathbb{K}_1 := \mathbb{P}(\mathscr{K}_1^\vee)$. By replacing $\mathscr{P}$ with $\mathscr{P} \otimes \pi_{\mathrm{Jac}^d}^\star$ (sufficiently ample)$^\vee$, we may assume that $\mathscr{O}_{\mathbb{K}_1}(1)$ is very ample. Let $\mathfrak{d}\colon \mathfrak{P} \longrightarrow \mathrm{Jac}^d$ be the morphism associated with $\bigwedge^r(E_{\mathfrak{P}})$, and let $\mathfrak{A}_{\mathfrak{P}}$ be a line bundle on $\mathfrak{P}$ with $\bigwedge^r(E_{\mathfrak{P}}) \cong (\mathfrak{d} \times \mathrm{id}_C)^\star(\mathscr{P}) \otimes \pi_{\mathfrak{P}}^\star(\mathfrak{A}_{\mathfrak{P}})$. Then,

$$\bigwedge^r\big(k_{\mathfrak{P}} \otimes \mathrm{id}_{\pi_C^\star(\mathscr{O}_C(n))}\big)\colon \bigwedge^r(Y) \otimes \mathscr{O}_{\mathfrak{P}} \longrightarrow (\mathfrak{d} \times \mathrm{id}_C)^\star(\mathscr{P}) \otimes \pi_C^\star\big(\mathscr{O}_C(rn)\big) \otimes \pi_{\mathfrak{P}}^\star(\mathfrak{A}_{\mathfrak{P}})$$

defines a morphism $\iota_1\colon \mathfrak{P} \longrightarrow \mathbb{K}_1$ with $\iota_1^\star(\mathscr{O}_{\mathbb{K}_1}(1)) \cong \mathfrak{A}_{\mathfrak{P}}$.
Define $\mathbb{K}_2 := \mathbb{P}(\mathscr{H}^\vee)$ (see above) as well as the *Gieseker space* $\mathbb{G} := \mathbb{K}_1 \times \mathbb{K}_2 \times \mathfrak{G}$, and let

$$\iota := (\iota_1 \times \mathrm{id}_{\mathbb{K}_2} \times \mathrm{id}_{\mathfrak{G}})\colon \mathfrak{P} \longrightarrow \mathbb{G}$$

be the natural, $\mathrm{SL}(Y)$-equivariant, and injective morphism. Using the ample line bundles on the $\mathfrak{G}_{ij}$ that are induced by the Plücker embedding, we find, for every tuple $\underline{e} := (e_1; e_2; \varepsilon_{ij}, j = 1, ..., t_i, i = 1, ..., s)$ of positive rational numbers, the $\mathrm{SL}(Y)$-linearized ample $\mathbb{Q}$-line bundle

$$\mathscr{L}_{\underline{e}} := \mathscr{O}\big(e_1; e_2; \varepsilon_{ij}, j = 1, ..., t_i, i = 1, ..., s\big)$$

on the Gieseker space $\mathbb{G}$.
Linearize the $\mathrm{SL}(Y)$-action on $\mathbb{G}$ in $\mathscr{L}_{\underline{e}}$ with

$$e_1 := l - u\cdot\delta - \sum_{i=1}^{s}\sum_{j=1}^{t_i} r_{ij}\cdot a_{ij}, \quad e_2 := r\cdot\delta, \quad \varepsilon_{ij} := r\cdot a_{ij},\ j = 1, ..., t_i,\ i = 1, ..., s, \tag{10}$$

and denote by $\mathbb{G}^{\underline{e}\text{-(s)s}}$ the sets of points in $\mathbb{G}$ that are $\mathrm{SL}(Y)$-(semi)stable with respect to the linearization in the line bundle $\mathscr{L}_{\underline{e}}$.

Theorem 5.6.1. *Given a point $p \in \mathfrak{P}$, denote by $(E_p; \underline{q}_p; \varphi_p)$ the restriction of the universal family to $\mathfrak{P} \times \{p\}$. Then, for n large enough, the following two properties hold true.*
i) *The preimages $\iota^{-1}(\mathbb{G}^{\underline{e}\text{-(s)s}})$ consist exactly of those points $p \in \mathfrak{P}$ for which $(E_p; \underline{q}_p; \varphi_p)$ is an $(\underline{a}, \delta)$-(semi)stable decorated flagged vector bundle of type $(r, d, \underline{x}, \underline{r}, u, v, L)$.*
ii) *The morphism*

$$\iota' : \mathfrak{P}^{\underline{e}\text{-ss}} \longrightarrow \mathbb{G}^{\underline{e}\text{-ss}},$$

induced by restricting the morphism ι to the preimage $\mathfrak{P}^{\underline{e}\text{-ss}}$ of $\mathbb{G}^{\underline{e}\text{-ss}}$, is proper.

The proof resembles the one of Theorem 2.11 in [37] and Theorem 4.4.1 in [15]. A part of it will be explained in the following section.

Elements of the Proof of Theorem 5.6.1. — Let p be a point in the parameter space $\mathfrak{P}$, such that the decorated flagged vector bundle $(E_p; \underline{q}_p; \varphi_p)$ is $(\underline{a}, \delta)$-(semi)stable. In this section, we will demonstrate that the Gieseker point $\iota(p)$ is (semi)stable with respect to the chosen linearization of the $\mathrm{SL}(Y)$-action.
By the Hilbert–Mumford criterion, we have to show that, for every one-parameter subgroup $\lambda\colon \mathbb{G}_m(k) \longrightarrow \mathrm{SL}(Y)$, the inequality

$$\begin{aligned} \mu_{\mathscr{L}_{\underline{e}}}\big(\lambda, \iota(p)\big) \quad &= \quad e_1 \cdot \mu_{\mathscr{O}_{\mathbb{K}_1}(1)}\big(\lambda, \iota_1(t)\big) + e_2 \cdot \mu_{\mathscr{O}_{\mathbb{K}_2}(1)}\big(\lambda, \iota_2(t)\big) \\ &\qquad + \sum_{i=1}^{s} \sum_{j=1}^{t_i} \varepsilon_{ij} \cdot \mu_{\mathscr{O}_{\mathfrak{G}_{ij}}(1)}(\lambda, q_{ij}) \quad (\geq) \quad 0 \end{aligned} \tag{11}$$

is satisfied. The one-parameter subgroup λ provides us with the weighted flag $(Y_\bullet(\lambda), \delta_\bullet(\lambda))$ in the vector space Y. We write

$$Y_\bullet(\lambda) : 0 =: Y_0 \subsetneq Y_1 \subsetneq \cdots \subsetneq Y_\tau \subsetneq Y_{\tau+1} := Y; \quad \delta_\bullet(\lambda) = (\delta_1, ..., \delta_\tau).$$

We remind the reader that there is an integer $N > 0$ (which is the number of summands in (5)), such that

$$\mathbb{D}^{u,v}(Y) \subset Y_{u,N} := \big(Y^{\otimes u}\big)^{\oplus N}.$$

Let $k_p\colon Y \otimes \mathscr{O}_C(-n) \longrightarrow E_p$ be the quotient corresponding to p. For $h \in \{1, ..., \tau\}$, define $l_h := \dim(Y_h)$ and $\mathscr{F}_h := k_p(Y_h \otimes \mathscr{O}_C(-n))$. Now, using (11), we compute

$$\begin{aligned} \mu_{\mathscr{L}_{\underline{e}}}\big(\lambda, \iota(p)\big) \quad &= \quad e_1 \cdot \sum_{h=1}^{\tau} \delta_h \cdot \big(l \cdot \mathrm{rk}(\mathscr{F}_h) - l_h \cdot r\big) + e_2 \cdot \mu_{\mathscr{O}_{\mathbb{K}_2}(1)}\big(\lambda, \iota_2(t)\big) + \\ &\qquad + \sum_{i=1}^{s} \sum_{j=1}^{t_i} \varepsilon_{ij} \cdot \sum_{h=1}^{\tau} \delta_h \cdot \big(l \cdot \dim(q_{ij}(\mathscr{F}_h)) - l_h \cdot r_{ij}\big). \end{aligned}$$

We first inspect the quantity $\mu_{\mathscr{O}_{\mathbb{K}_2}(1)}(\lambda, \iota_2(t))$. To this end, let $\widetilde{E}_h$ be the subbundle of E_p that is generated by $\mathscr{F}_h$, $h = 0, ..., \tau + 1$. Note that improper inclusions may occur among the bundles $\widetilde{E}_h$, i.e., there might exist indices $h' < h$ with $\widetilde{E}_{h'} = \widetilde{E}_h$. We eliminate these improper inclusions in order to find the filtration

$$E_\bullet : 0 =: E_0 \subsetneq E_1 \subsetneq \cdots \subsetneq E_t \subsetneq E_{t+1} := E_p.$$

With each index $j \in \{ 1, ..., t \}$, we associate the set

$$T(j) := \Big\{ h \in \{ 1, ..., \tau \} \,\Big|\, \widetilde{E}_h = E_j \Big\}$$

and the positive rational number

$$\beta_j := \sum_{h \in T(j)} \delta_h. \tag{12}$$

Setting $\beta_\bullet := (\beta_1, ..., \beta_t)$, we have defined the weighted filtration $(E_\bullet, \beta_\bullet)$ of E. In addition, we define the function $J \colon \{ 1, ..., \tau \} \longrightarrow \{ 1, ..., t \}$ by requiring that $\widetilde{E}_h = E_{J(h)}$, $h = 1, ..., \tau$. For an index $j \in \{ 0, ..., t+1 \}$, we set

$$\begin{array}{rcl} \underline{h}(j) & := & \min\big\{ h = 1, ..., \tau \,|\, \widetilde{E}_h = E_j \big\}, \quad \underline{Y}_j := Y_{\underline{h}(j)}, \\ \overline{h}(j) & := & \max\big\{ h = 1, ..., \tau \,|\, \widetilde{E}_h = E_j \big\}, \quad \overline{Y}_j := Y_{\overline{h}(j)}, \end{array}$$

and also, for $j = 1, ..., t$,

$$\widetilde{Y}_j := \underline{Y}_j / \overline{Y}_{j-1}.$$

Next, given an index tuple $(i_1, ..., i_u) \in I := \{ 1, ..., t+1 \}^{\times u}$, we introduce the vector space

$$\widetilde{Y}_{i_1,\dots,i_u} := \big(\widetilde{Y}_{i_1} \otimes \cdots \otimes \widetilde{Y}_{i_u}\big)^{\oplus N}.$$

We fix a basis $\underline{y}$ for Y that consists of eigenvectors for the one-parameter subgroup λ and has the property

$$\langle\, y_1, ..., y_{l_h} \,\rangle = Y_h, \quad h = 0, ..., \tau + 1.$$

Using this basis, we may view $(\widetilde{Y}_{i_1,\dots,i_u})^{\oplus N}$ as a subspace of $Y_{\nu,N}$, and declare

$$\widetilde{Y}^\star_{i_1,\dots,i_u} := \widetilde{Y}_{i_1,\dots,i_u} \cap \mathbb{D}^{u,v}(Y).$$

If we are also given a weight vector $\underline{\gamma} = (\gamma_1, ..., \gamma_l)$, we let $\lambda(\underline{y}, \underline{\gamma})$ be the one-parameter subgroup with $\lambda(\underline{y}, \underline{\gamma})(y_i) = z^{\gamma_i} \cdot y_i$, $z \in \mathbb{G}_m(k)$, $i = 1, ..., l$. Apparently,

$$\lambda = \lambda(\underline{y}, \underline{\gamma}) \quad \text{for } \underline{\gamma} = \sum_{h=1}^{\tau} \delta_h \cdot \gamma_l^{(l_h)}.$$

We also define the one-parameter subgroups $\lambda^h := \lambda(\underline{y}, \gamma_l^{(l_h)})$, $h = 1, ..., \tau$. Then, the subspaces $\widetilde{Y}^\star_{i_1,\dots,i_u}$, $(i_1, ..., i_u) \in I$, that we have just defined are eigenspaces for all the one-parameter subgroups $\lambda^1, ..., \lambda^\tau$. Indeed, define for $\underline{i} \in I$ and $j \in \{0, ..., t+1\}$,

$$\nu_j(\underline{i}) = \#\{ i_k \leq j \,|\, k = 1, ..., u \}.$$

Since $\underline{h}(j) \leq h$ holds precisely when $j \leq J(h)$, the one-parameter subgroup λ^h acts on $\widetilde{Y}^\star_{i_1,...,i_u}$ with weight $l_h \cdot u - l \cdot \nu_{J(h)}(i_1, ..., i_u)$, $\underline{i} = (i_1, ..., i_u) \in I$, $h = 1, ..., \tau$.
The homomorphism φ_p is determined by the homomorphism

$$F_p \colon \mathbb{D}^{u,v}(Y) \longrightarrow H^0\big(L(un)\big).$$

Therefore,

$$\mu_{\mathscr{O}_{\mathbb{K}_2(1)}}(\lambda, F_p) \geq \tag{13}$$
$$-\min\Big\{ \sum_{h=1}^{\tau} \delta_h\big(l_h \cdot u - l \cdot \nu_{J(h)}(i_1, ..., i_u)\big) \,\big|\, \underline{i} = (i_1, ..., i_u) \in I : F_{p|\widetilde{Y}^\star_{i_1,...,i_u}} \not\equiv 0 \Big\}.$$

Let $\underline{i}_0 = (i^0_1, ..., i^0_u) \in I$ be an index tuple, such that the minimum in the second formula in Remark 5.1.9 is achieved for this index tuple.

LEMMA 5.6.2. *The restricted homomorphism $F_{p|\widetilde{Y}^\star_{i^0_1,...,i^0_u}}$ is non-trivial.*

Proof. Under the surjection $\mathbb{D}^{u,v}(Y \otimes \mathscr{O}_C(n)) \longrightarrow \mathbb{D}^{u,v}(E_p(n))$ that is induced by k_p, the vector space $F_{p|\widetilde{Y}^\star_{i^0_1,...,i^0_u}}$ maps to the global sections of the bundle $E_{i^0_1}(n) \star \cdots \star E_{i^0_u}(n)$, and

$$\Big(\mathbb{D}^{u,v}(Y) \cap \big(Y'_{i^0_1} \otimes \cdots \otimes Y'_{i^0_u}\big)^{\oplus N} \Big) \otimes \mathscr{O}_C(un) \quad \text{with } Y'_j := \bigoplus_{k=1}^{j} \widetilde{Y}_k,\ j = 1, ..., t,$$

generically generates that bundle. To see these assertions, observe that

$$D^{u_1}(Y) \otimes \cdots \otimes D^{u_v}(Y) \subset Y^{\otimes u}, \text{ for } u_1 + \cdots + u_v = u,$$

is, by definition, the submodule that is invariant under action of $\Sigma_{u_1} \times \cdots \times \Sigma_{u_v}$, Σ_w being the symmetric group in w letters, $w > 0$. The intersection

$$D^{u_1}(Y) \otimes \cdots \otimes D^{u_v}(Y) \cap \big(Y'_{i^0_1} \otimes \cdots \otimes Y'_{i^0_u}\big)$$

is consequently of the form

$$D^{u_1}(Y'_{i^\star_1}) \otimes \cdots \otimes D^{u_v}(Y'_{i^\star_v})$$

where $i^\star_1$ is the smallest index among $i^0_1,...,i^0_{u_1}$, $i^\star_2$ is the smallest index among $i^0_{u_1+1},...,i^0_{u_2}$, and so on. The map $(Y \otimes \mathscr{O}_C(-n))^{\otimes u} \longrightarrow E_p^{\otimes u}$ is certainly equivariant under the $(\Sigma_{u_1} \times \cdots \times \Sigma_{u_v})$-action and is easily seen to induce a surjection

$D^{u_1}(Y\otimes\mathscr{O}_C(-n))\otimes\cdots\otimes D^{u_v}(Y\otimes\mathscr{O}_C(-n))\longrightarrow D^{u_1}(E_p)\otimes\cdots\otimes D^{u_v}(E_p)$. Since the isomorphism $Y\longrightarrow H^0(E_p(n))$ maps Y'_j to the global sections of $E_j(n)$, $j=1,...,t$, and Y'_j generically generates the bundle E_j, we see that $D^{u_1}(Y'_{i_1^\star})\otimes\cdots\otimes D^{u_v}(Y'_{i_v^\star})$ generically generates

$$D^{u_1}(E_{i_1^\star})\otimes\cdots\otimes D^{u_v}(E_{i_v^\star})=\big(D^{u_1}(E_p)\otimes\cdots\otimes D^{u_v}(E_p)\big)\cap\big(E_{i_1^0}\otimes\cdots\otimes E_{i_u^0}\big).$$

Therefore, if $F_{p|\widetilde{Y}^\star_{i_1^0,...,i_u^0}}$ were zero, we would find indices $i'_j\le i_j^0$, $j=1,...,u$, where at least one inequality is strict, such that $F_{p|\widetilde{Y}^\star_{i'_1,...,i'_u}}\not\equiv 0$. By the same argument as before, this would imply that the restriction of φ_p to $E_{i'_1}\star\cdots\star E_{i'_u}$ was non-trivial. But clearly

$$\gamma_{i'_1}+\cdots+\gamma_{i'_u}<\gamma_{i_1^0}+\cdots+\gamma_{i_u^0}.$$

This contradicts our choice of $\underline{i}_0$. □

Using (13), we find

$$\begin{aligned}\mu_{\mathscr{O}_{\mathbb{K}_2(1)}}(\lambda,F_p) &\ge -\sum_{h=1}^{\tau}\delta_h\cdot\big(l_h\cdot u-l\cdot\nu_{J(h)}(i_1^0,...,i_u^0)\big)\\ &\ge -\sum_{j=1}^{t}\beta_j\cdot\big(h^0(E_j(n))\cdot u-l\cdot\nu_j(i_1^0,...,i_u^0)\big). \qquad (14)\end{aligned}$$

We note our first estimate:

$$\begin{aligned}\mu_{\mathscr{L}_{\underline{e}}}\big(\lambda,\iota(p)\big) \ge\ & e_1\cdot\sum_{h=1}^{\tau}\delta_h\cdot\big(l\cdot\mathrm{rk}(\mathscr{F}_h)-l_h\cdot r\big)+\\ &+e_2\cdot\sum_{j=1}^{t}\beta_j\cdot\big(l\cdot\nu_j(i_1^0,...,i_u^0)-h^0(E_j(n))\cdot u\big)+ \qquad (15)\\ &+\sum_{i=1}^{s}\sum_{j=1}^{t_i}\varepsilon_{ij}\cdot\sum_{h=1}^{\tau}\delta_h\cdot\big(l\cdot\dim(q_{ij}(\mathscr{F}_h))-l_h\cdot r_{ij}\big).\end{aligned}$$

For $j\in\{1,...,t\}$, choose $h^\star(j)\in T(j)$, such that

$$\begin{aligned}&e_1\cdot\big(l\cdot\mathrm{rk}(\mathscr{F}_{h^\star(j)})-l_{h^\star(j)}\cdot r\big)+\\ &\quad+\sum_{i=1}^{s}\sum_{j=1}^{t_i}\varepsilon_{ij}\cdot\big(l\cdot\dim(q_{ij}(\mathscr{F}_{h^\star(j)}))-l_{h^\star(j)}\cdot r_{ij}\big)\\ &=\min\Big\{e_1\cdot\big(l\cdot\mathrm{rk}(\mathscr{F}_h)-l_h\cdot r\big)+\sum_{i=1}^{s}\sum_{j=1}^{t_i}\varepsilon_{ij}\cdot\big(l\cdot\dim(q_{ij}(\mathscr{F}_h))-l_h\cdot r_{ij}\big)\ \Big|\\ &\qquad\qquad h\in T(j)\Big\}.\end{aligned}$$

Together with (15), we arrive at our second estimate:

$$\begin{aligned}\mu_{\mathscr{L}_{\underline{e}}}\big(\lambda,\iota(p)\big) \quad \geq \quad & e_1\cdot\sum_{k=1}^{t}\beta_k\cdot\big(l\cdot \mathrm{rk}(\mathscr{F}_{h^\star(k)})-l_{h^\star(k)}\cdot r\big)+\\ & +e_2\cdot\sum_{k=1}^{t}\beta_k\cdot\big(l\cdot v_k(\underline{i}_0)-h^0(E_k(n))\cdot u\big)+\\ & +\sum_{i=1}^{s}\sum_{j=1}^{t_i}\varepsilon_{ij}\cdot\sum_{k=1}^{t}\beta_k\cdot\big(l\cdot\dim(q_{ij}(\mathscr{F}_{h^\star(k)}))-l_{h^\star(k)}\cdot r_{ij}\big).\end{aligned} \tag{16}$$

Plugging in the definition (10) of the linearization parameters, Formula (16) transforms into

$$\begin{aligned}& \mu_{\mathscr{L}_{\underline{e}}}\big(\lambda,\iota(p)\big)\\ \geq\quad & \sum_{k=1}^{t}\beta_k\cdot\Big(l^2\cdot\mathrm{rk}(\mathscr{F}_{h^\star(k)})-l\cdot u\cdot\delta\cdot\mathrm{rk}(\mathscr{F}_{h^\star(k)})-\\ & -l\cdot\sum_{i=1}^{s}\sum_{j=1}^{t_i}r_{ij}\cdot a_{ij}\cdot\mathrm{rk}(\mathscr{F}_{h^\star(k)})-l\cdot l_{h^\star(k)}\cdot r\Big)+\\ & +r\cdot\delta\cdot\sum_{k=1}^{t}\beta_k\cdot l\cdot\nu_k(\underline{i}_0)+r\cdot\sum_{i=1}^{s}\sum_{j=1}^{t_i}a_{ij}\cdot\sum_{k=1}^{t}\beta_k\cdot l\cdot\dim(q_{ij}(\mathscr{F}_{h^\star(k)})).\end{aligned}$$

Note that $l_{h^\star(k)}\leq h^0(\mathscr{F}_{h^\star(k)}(n))$, so that we find

$$\begin{aligned}& \mu_{\mathscr{L}_{\underline{e}}}\big(\lambda,\iota(p)\big)\\ \geq\quad & \sum_{k=1}^{t}\beta_k\Big(l^2\cdot\mathrm{rk}(\mathscr{F}_{h^\star(k)})-l\cdot u\cdot\delta\cdot\mathrm{rk}(\mathscr{F}_{h^\star(k)})-\\ & -l\cdot\sum_{i=1}^{s}\sum_{j=1}^{t_i}r_{ij}\cdot a_{ij}\cdot\mathrm{rk}(\mathscr{F}_{h^\star(k)})-l\cdot h^0(\mathscr{F}_{h^\star(k)}(n))\cdot r\Big)+\\ & +r\cdot\delta\cdot\sum_{k=1}^{t}\beta_k\cdot l\cdot\nu_k(\underline{i}_0)+r\cdot\sum_{i=1}^{s}\sum_{j=1}^{t_i}a_{ij}\cdot\sum_{k=1}^{t}\beta_k\cdot l\cdot\dim(q_{ij}(\mathscr{F}_{h^\star(k)})).\end{aligned}$$

We divide the quantity on the right hand side by l and rearrange it, until we get

$$\begin{aligned}\mu_{\mathscr{L}_{\underline{e}}}\big(\lambda,\iota(p)\big) \quad \geq \quad & \sum_{k=1}^{t}\beta_k\cdot\big(l\cdot \mathrm{rk}(\mathscr{F}_{h^\star(k)})-h^0(\mathscr{F}_{h^\star(k)}(n))\cdot r\big)+\\ &+\delta\cdot\sum_{k=1}^{t}\beta_k\cdot\big(r\cdot\nu_k(\underline{i}_0)-u\cdot\mathrm{rk}(E_k)\big)+ \qquad (17)\\ &+\sum_{i=1}^{s}\sum_{j=1}^{t_i}a_{ij}\sum_{k=1}^{t}\beta_k\big(r\cdot\dim(q_{ij}(\mathscr{F}_{h^\star(k)}))-\mathrm{rk}(\mathscr{F}_{h^\star(k)})\cdot r_{ij}\big).\end{aligned}$$

By our choice of $\underline{i}_0$, the number $\sum_{k=1}^t \beta_k\cdot(r\cdot\nu_k(\underline{i}_0)-u\cdot \mathrm{rk}(E_k))$ equals $\mu(E_\bullet,\beta_\bullet;\varphi_p)$. Our contention is therefore a consequence of the next result.

Proposition 5.6.3. *Having fixed the input data r, d, u, v, and L, as well as the stability parameters $\underline{a}$ and δ, there exists an n_1, such that any $(\underline{a},\delta)$-(semi)stable decorated flagged vector bundle (E,L,φ) of type $(r,d,\underline{x},\underline{r},u,v,L)$ has the following property: Let*

$$0\subsetneq \mathscr{F}_1\subsetneq\cdots\subsetneq\mathscr{F}_t\subsetneq E$$

be a filtration of E by not necessarily saturated subsheaves, such that $0<\mathrm{rk}(\mathscr{F}_1)<\cdots<\mathrm{rk}(\mathscr{F}_t)<r$, let

$$E_\bullet: 0\subsetneq E_1\subsetneq\cdots\subsetneq E_t\subsetneq E$$

be the filtration of E by the subbundles $E_i:=\ker(E\longrightarrow (E/\mathscr{F}_i)/\mathrm{Torsion}(E/\mathscr{F}_i))$, $i=1,...,t$, and let $\beta_\bullet=(\beta_1,...,\beta_t)$ be a tuple of positive rational numbers. Then, for all $n\geq n_1$,

$$\begin{aligned}0\quad\leq\quad & \sum_{k=1}^{t}\beta_k\cdot\big(h^0(E(n))\cdot\mathrm{rk}(\mathscr{F}_k)-h^0(\mathscr{F}_k(n))\cdot r\big)+\delta\cdot\mu(E_\bullet,\beta_\bullet;\varphi)+\\ &+\sum_{i=1}^{s}\sum_{j=1}^{t_i}a_{ij}\cdot\sum_{k=1}^{t}\beta_k\cdot\big(r\cdot\dim(q_{ij}(\mathscr{F}_k))-\mathrm{rk}(\mathscr{F}_k)\cdot r_{ij}\big).\end{aligned}$$

Proof. We choose $n_1\geq n_0$, so that $h^1(E(n))=0$ and $l:=h^0(E(n))=d+r(n+1-g)$. First, we assume that the sheaves $\mathscr{F}_1(n),...,\mathscr{F}_t(n)$ are all globally generated and have trivial first cohomology spaces. The same holds then for $E_1(n)$,...,$E_t(n)$. Let $\mathscr{T}_i$ be the torsion sheaf $E_i/\mathscr{F}_i$, $i=1,...,t$. Since $H^1(\mathscr{F}_i(n))=\{0\}$, the map $H^0(E_i(n))\longrightarrow\mathscr{T}_i$ is surjective, so that

$$h^0\big(E_i(n)\big)=h^0\big(\mathscr{F}_i(n)\big)+\dim(\mathscr{T}_i),\quad i=1,...,t. \qquad (18)$$

Invoking $\sum_{j=1}^{t_i}a_{ij}<1$, $i=1,...,s$, once more, we discover

$$\sum_{j=1}^{t_i}a_{ij}\cdot\dim(q_{ij}(E_k))\leq\sum_{j=1}^{t_i}a_{ij}\cdot\dim(q_{ij}(\mathscr{F}_k))+\dim(\mathscr{T}_{k|\{x_i\}}),\quad i=1,...,s.$$

In this case, we consequently find

$$
\begin{aligned}
& \sum_{k=1}^{t} \beta_k \cdot \big(h^0(E(n)) \cdot \mathrm{rk}(E_k) - h^0(\mathscr{F}_k(n)) \cdot r\big) + \delta \cdot \mu(E_\bullet, \beta_\bullet; \varphi) + \\
& + \sum_{i=1}^{s} \sum_{j=1}^{t_i} a_{ij} \cdot \sum_{k=1}^{t} \beta_k \cdot \big(r \cdot \dim(q_{ij}(\mathscr{F}_k)) - \mathrm{rk}(\mathscr{F}_k) \cdot r_{ij}\big) \\
\geq \; & \sum_{k=1}^{t} \beta_k \cdot \big(h^0(E(n)) \cdot \mathrm{rk}(E_k) - h^0(E_k(n)) \cdot r\big) + \delta \cdot \mu(E_\bullet, \beta_\bullet; \varphi) + \\
& + \sum_{i=1}^{s} \sum_{j=1}^{t_i} a_{ij} \cdot \sum_{k=1}^{t} \beta_k \cdot \big(r \cdot \dim(q_{ij}(E_k)) - \mathrm{rk}(E_k) \cdot r_{ij}\big) \qquad (19) \\
= \; & \sum_{k=1}^{t} \beta_k \cdot \big(\deg(E) \cdot \mathrm{rk}(E_k) - \deg(E_k) \cdot r\big) + \delta \cdot \mu(E_\bullet, \beta_\bullet; \varphi) + \\
& + \sum_{i=1}^{s} \sum_{j=1}^{t_i} a_{ij} \cdot \sum_{k=1}^{t} \beta_k \cdot \big(r \cdot \dim(q_{ij}(E_k)) - \mathrm{rk}(E_k) \cdot r_{ij}\big) \\
= \; & M_{\underline{a}}(E_\bullet, \beta_\bullet) + \delta \cdot \mu(E_\bullet, \beta_\bullet; \varphi) \quad (\geq) \quad 0.
\end{aligned}
$$

Let $\mathfrak{S}$ be the bounded family of isomorphism classes of locally free sheaves E of rank r and degree d on C for which there exists an $(\underline{a}, \delta)$-semistable decorated flagged vector bundle $(E, \underline{q}, \varphi)$ of type $(r, d, \underline{x}, \underline{r}, u, v, L)$. Suppose that we have fixed some positive constant K. Then, we divide the locally free sheaves $\mathscr{F}$ on C that may occur as subsheaves of sheaves in the family $\mathfrak{S}$ into two classes:

A. $\mu(\mathscr{F}) \geq d/r - K$

B. $\mu(\mathscr{F}) < d/r - K$.

By the Langer–LePotier–Simpson estimate [28], there are non-negative constants K_1 and K_2 which depend only on r, such that any locally free $\mathscr{O}_C$-module A on C of rank at most r satisfies

$$
\begin{aligned}
& h^0(A) \leq \\
& \mathrm{rk}(A) \cdot \left(\frac{\mathrm{rk}(A) - 1}{\mathrm{rk}(A)} \cdot \big[\mu_{\max}(A) + K_1 + 1\big]_+ + \frac{1}{\mathrm{rk}(A)} \cdot \big[\mu(A) + K_2 + 1\big]_+ \right).
\end{aligned}
$$

For a sheaf A in Class B, this leads to

$$
h^0\big(A(n)\big) \leq \mathrm{rk}(A) \cdot \left(\frac{d}{r} + n + 1 + (r-1)(K_0 + K_1) + K_2 - \frac{1}{r} \cdot K \right),
$$

if the right hand side is positive. There exists an integer $n'(K) = n'(r, d, K_1, K_2, K)$ such that this holds for $n \geq n'(K)$. Furthermore, we estimate

$$
\begin{aligned}
& h^0(E(n)) \cdot \mathrm{rk}(A) - h^0(A(n)) \cdot r \geq \\
& \quad -(r-1)rg - (r-2)(r-1)r(K_0 + K_1) - (r-2)rK_2 + K =: L.
\end{aligned}
$$

We choose K so large that

$$L \geq \delta \cdot u \cdot (r-1) + \Bigl(\sum_{i=1}^{s}\sum_{j=1}^{t_i} a_{ij}\Bigr) \cdot (r-1)^2.$$

Suppose that all the sheaves $\mathscr{F}_1, ..., \mathscr{F}_t$ belong to Class B. Then,

$$\begin{aligned} & \sum_{k=1}^{t} \beta_k \cdot \bigl(h^0(E(n)) \cdot \mathrm{rk}(\mathscr{F}_k) - h^0(\mathscr{F}_k(n)) \cdot r\bigr) - \delta \cdot u \cdot (r-1) \cdot \sum_{k=1}^{l} \beta_k + \\ & + \sum_{i=1}^{s}\sum_{j=1}^{t_i} a_{ij} \cdot \sum_{k=1}^{t} \beta_k \cdot \bigl(r \cdot \dim(q_{ij}(\mathscr{F}_k)) - \mathrm{rk}(\mathscr{F}_k) \cdot r_{ij}\bigr) \\ \geq \;& \sum_{k=1}^{l} \beta_k \cdot \bigl(L - \delta \cdot u \cdot (r-1)\bigr) - \sum_{i=1}^{s}\sum_{j=1}^{t_i} a_{ij} \cdot \sum_{k=1}^{t} \beta_k \cdot \mathrm{rk}(E_k) \cdot r_{ij} \qquad (20) \\ \geq \;& \sum_{k=1}^{l} \beta_k \cdot \Bigl(L - \delta \cdot u \cdot (r-1) - (r-1)^2 \cdot \Bigl(\sum_{i=1}^{s}\sum_{j=1}^{t_i} a_{ij}\Bigr)\Bigr) \quad > \quad 0. \end{aligned}$$

Note that the sheaves in Class A form a bounded family: the ranks and degrees of those sheaves belong to finite sets and their $\mu_{\max}$ is bounded by $\mu_{\max}(E)$, $[E] \in \mathfrak{S}$. Hence, there is an $n''(K)$, such that, for any $n \geq n''(K)$ and any sheaf A of Class A, one finds that $A(n)$ is globally generated and that $h^1(A(n)) = 0$. Set $n_1 := \max\{\, n'(K), n''(K)\,\}$. We have to verify our assertion. To do so, we set $I := \{\, 1, ..., t\,\}$, $I_{\mathrm{A}} := \{\, i \in I \,|\, \mathscr{F}_i \text{ is in Class A}\,\}$, and $I_{\mathrm{B}} := \{\, i \in I \,|\, \mathscr{F}_i \text{ is in Class B}\,\}$, so that $I = I_{\mathrm{A}} \sqcup I_{\mathrm{B}}$. Write $I_{\mathrm{A/B}} = \{\, i_1^{\mathrm{A/B}}, ..., i_{t_{\mathrm{A/B}}}^{\mathrm{A/B}}\,\}$ with $i_1^{\mathrm{A/B}} < \cdots < i_{t_{\mathrm{A/B}}}^{\mathrm{A/B}}$. This gives the weighted filtrations

$$\bigl(E_\bullet^{\mathrm{A/B}} : 0 \subsetneq E_{i_1^{\mathrm{A/B}}} \subsetneq \cdots \subsetneq E_{i_{t_{\mathrm{A/B}}}^{\mathrm{A/B}}} \subsetneq E, \beta_\bullet^{\mathrm{A/B}} = (\beta_{i_1^{\mathrm{A/B}}}, ..., \beta_{i_{t_{\mathrm{A/B}}}^{\mathrm{A/B}}})\bigr).$$

It is then easy to see that

$$\mu\bigl(E_\bullet, \beta_\bullet; \varphi\bigr) \geq \mu\bigl(E_\bullet^{\mathrm{A}}, \beta_\bullet^{\mathrm{A}}; \varphi\bigr) - u \cdot (r-1) \cdot \sum_{j=1}^{t_{\mathrm{B}}} \beta_{i_j^{\mathrm{B}}}. \qquad (21)$$

Equation (21) together with the formulae (19) and (20) finally establishes the contention of the Proposition. □

The Remaining Steps. — The converse assertion, namely the fact that $(E_p, \underline{q}_p, \varphi_p)$ is $(\underline{a}, \delta)$-(semi)stable, if the Gieseker point associated with p is (semi)stable with respect to the linearization in $\mathscr{L}_{\underline{e}}$, is proved along similar lines, but is easier. The same holds for the proof of properness of the Gieseker map. The reader should combine the above arguments with those from [37] and [15] to fill in the details.

5.7 Construction of the Parameter Spaces for ϱ-Flagged Pseudo G-Bundles

We next include the explicit construction of the parameter space $\mathfrak{F}_{\varrho\text{-FLPsBun}}$ that will make the asserted properties in Proposition 5.3.1 evident.
There is a quasi-projective quot scheme $\mathfrak{Q}$ which parameterizes quotients $k\colon Y\otimes \mathscr{O}_C(-n)\longrightarrow E$ where E is a vector bundle of rank r and degree zero, such that $\mu_{\max}(E)\leq D$, and where $H^0(k(n))$ is an isomorphism. The scheme $\mathfrak{Q}\times C$ carries the *universal quotient*

$$k_{\mathfrak{Q}}\colon Y\otimes \pi_C^\star\big(\mathscr{O}_C(-n)\big)\longrightarrow E_{\mathfrak{Q}}.$$

For the vector bundle $E_{\mathfrak{Q}}$, as for any vector bundle of rank r, we have the canonical isomorphism

$$E_{\mathfrak{Q}}^\vee \cong \bigwedge^{r-1}(E_{\mathfrak{Q}})\otimes\Big(\bigwedge^{r}(E_{\mathfrak{Q}})\Big)^\vee.$$

Since the restriction of $(\bigwedge^r(E_{\mathfrak{Q}}))^\vee$ to any fiber $\{k\}\times C$, $k\in\mathfrak{Q}$, is trivial, there is a line bundle $\mathscr{A}$ on $\mathfrak{Q}$, such that

$$\Big(\bigwedge^{r}(E_{\mathfrak{Q}})\Big)^\vee\cong \pi_{\mathfrak{Q}}^\star(\mathscr{A}).$$

Gathering all this information, we find a surjection

$$\mathscr{S}\!ym^\star\Big(V\otimes\bigwedge^{r-1}\big(Y\otimes\pi_C^\star(\mathscr{O}_C(-n))\big)\otimes\pi_{\mathfrak{Q}}^\star(\mathscr{A})\Big)^G\longrightarrow \mathscr{S}\!ym^\star\big(V\otimes E_{\mathfrak{Q}}^\vee\big)^G.$$

For a point $[q\colon Y\otimes\mathscr{O}_C(-n)\longrightarrow E]\in\mathfrak{Q}$, any homomorphism $\tau\colon \mathscr{S}\!ym^\star(V\otimes E^\vee)^G\longrightarrow\mathscr{O}_C$ of $\mathscr{O}_C$-algebras is determined by the composite homomorphism

$$\bigoplus_{i=1}^{s}\mathscr{S}\!ym^i\Big(V\otimes\bigwedge^{r-1}\big(Y\otimes\mathscr{O}_C(-n)\big)\Big)^G\longrightarrow\mathscr{O}_C$$

of $\mathscr{O}_C$-modules. Noting that

$$\mathscr{S}\!ym^i\Big(V\otimes\bigwedge^{r-1}\big(Y\otimes\mathscr{O}_C(-n)\big)\Big)^G\cong \operatorname{Sym}^i\Big(V\otimes\bigwedge^{r-1}Y\Big)^G\otimes\mathscr{O}_C\big(-i(r-1)n\big),$$

τ is determined by a collection of homomorphisms

$$\varphi_i\colon \operatorname{Sym}^i\Big(V\otimes\bigwedge^{r-1}Y\Big)^G\otimes\mathscr{O}_C\longrightarrow\mathscr{O}_C\big(i(r-1)n\big),\quad i=1,...,s.$$

Since φ_i is determined by the induced linear map on global sections, we will construct the parameter space inside

$$\overline{\mathfrak{Y}}:=\bigoplus_{i=1}^{s}\mathscr{H}\!om\bigg(\mathscr{S}\!ym^i\Big(V\otimes\bigwedge^{r-1}Y\otimes\pi_{\mathfrak{Q}}^\star(\mathscr{A})\Big)^G,H^0\Big(\mathscr{O}_C\big(i(r-1)n\big)\Big)\otimes\mathscr{O}_{\mathfrak{Q}}\bigg).$$

Write $\pi\colon \overline{\mathfrak{Y}} \longrightarrow \mathfrak{Q}$ for the bundle projection and observe that, over $\overline{\mathfrak{Y}} \times C$, there are universal homomorphisms

$$\widetilde{\varphi}^i\colon \mathscr{S}ym^i\Big(V\otimes \bigwedge^{r-1} Y\otimes \big(\pi_{\mathfrak{Q}}\circ(\pi\times \mathrm{id}_C)\big)^\star(\mathscr{A})\Big)^G \to H^0\Big(\mathscr{O}_C\big(i(r-1)n\big)\Big)\otimes \mathscr{O}_{\overline{\mathfrak{Y}}\times C},\cdot$$

$i = 1, ..., s$. Define $\varphi^i = \mathrm{ev}\circ\widetilde{\varphi}^i$ as the composition of $\widetilde{\varphi}^i$ with the evaluation map $\mathrm{ev}\colon H^0(\mathscr{O}_C(i(r-1)n))\otimes\mathscr{O}_{\overline{\mathfrak{Y}}\times C} \longrightarrow \pi_C^\star(\mathscr{O}_C(i(r-1)n))$, $i = 1, ..., s$. We twist φ^i by $\mathrm{id}_{\pi_C^\star(\mathscr{O}_C(-i(r-1)n))}$ and put the resulting maps together to obtain the homomorphism

$$\varphi\colon \mathscr{V}_{\overline{\mathfrak{Y}}} \longrightarrow \mathscr{O}_{\overline{\mathfrak{Y}}\times C}$$

with

$$\mathscr{V}_{\overline{\mathfrak{Y}}} := \bigoplus_{i=1}^s \mathscr{S}ym^i\Big(V\otimes \bigwedge^{r-1}\Big(Y\otimes \pi_C^\star\big(\mathscr{O}_C(-n)\big)\Big)\otimes \big(\pi_{\mathfrak{Q}}\circ(\pi\times\mathrm{id}_C)\big)^\star(\mathscr{A})\Big)^G.$$

Next, φ yields a homomorphism of $\mathscr{O}_{\overline{\mathfrak{Y}}\times C}$-algebras

$$\widetilde{\tau}_{\overline{\mathfrak{Y}}}\colon \mathscr{S}ym^\star\big(\mathscr{V}_{\overline{\mathfrak{Y}}}\big) \longrightarrow \mathscr{O}_{\overline{\mathfrak{Y}}\times C}.$$

On the other hand, there is a surjective homomorphism

$$\beta\colon \mathscr{S}ym^\star(\mathscr{V}_{\overline{\mathfrak{Y}}}) \longrightarrow \mathscr{S}ym^\star\Big(V\otimes(\pi\times\mathrm{id}_C)^\star\big(E_{\mathfrak{Q}}^\vee\big)\Big)^G$$

of graded algebras where the left hand algebra is graded by assigning the weight i to the elements in $\mathscr{S}ym^i(\cdots)^G$. The parameter space $\mathfrak{Y}$ is defined by the condition that $\widetilde{\tau}_{\overline{\mathfrak{Y}}}$ factorizes over β, i.e., setting $E_{\mathfrak{Y}} := ((\pi\times\mathrm{id}_C)^\star(E_{\mathfrak{Q}}))_{|\mathfrak{Y}\times C}$, there is a homomorphism

$$\tau_{\mathfrak{Y}}\colon \mathscr{S}ym^\star\big(V\otimes E_{\mathfrak{Y}}^\vee\big)^G \longrightarrow \mathscr{O}_{\mathfrak{Y}\times C}$$

with $\widetilde{\tau}_{\overline{\mathfrak{Y}}|\mathfrak{Y}\times C} = \tau_{\mathfrak{Y}}\circ\beta$. Formally, $\mathfrak{Y}$ is defined as the scheme theoretic intersection of the closed subschemes

$$\mathfrak{Y}_d := \Big\{\, y\in\overline{\mathfrak{Y}}\;\big|\; \widetilde{\tau}^d_{\overline{\mathfrak{Y}}|\{y\}\times C}\colon \ker\big(\beta^d_{|\{y\}\times C}\big) \longrightarrow \mathscr{O}_C \text{ is trivial}\Big\},\quad d\geq 0.$$

The family $(E_{\mathfrak{Y}}, \tau_{\mathfrak{Y}})$ is the *universal family of pseudo G-bundles parameterized by $\mathfrak{Y}$*.

Remark 5.7.1. i) The scheme $\mathfrak{Y}$ is equipped with a natural $\mathrm{GL}(Y)$-action, and the vector bundle $E_{\mathfrak{Y}}$ is linearized with respect to this group action.
ii) Note that elimination theory shows that there is an open subscheme $\mathfrak{Y}^0$ that parameterizes the principal G-bundles. Moreover, there exists a *universal principal G-bundle* $\mathscr{P}_{\mathfrak{Y}^0}$ on $\mathfrak{Y}^0\times C$.
iii) There is a locally closed and $\mathrm{GL}(Y)$-invariant subscheme $\mathfrak{Y}^{\vartheta,\geq h}\subset\mathfrak{Y}^0$ which parameterizes those principal G-bundles $\mathscr{P}$ that have topological type ϑ and instability degree at least h. By construction, every such principal bundle $\mathscr{P}$ is represented by at least one point in $\mathfrak{Y}^{\vartheta,\geq h}$, so that we have a surjective map $\mathfrak{Y}^{\vartheta,\geq h}\longrightarrow \mathrm{Bun}_G^{\vartheta,\geq h}$. In fact, this map identifies $\mathrm{Bun}_G^{\vartheta,\geq h}$ with the quotient $[\mathfrak{Y}^{\vartheta,\geq h}/\,\mathrm{GL}(Y)]$.

We proceed to parameterize ϱ-flagged pseudo G-bundles. For this, we fix the tuple $\underline{x} = (x_1, ..., x_b)$ of points on C and the type $\underline{r} = (r_{ij}, j = 1, ..., t_i, i = 1, ..., b)$ of the flaggings. The tuple $(r_{i1}, ..., r_{it_i})$ determines the conjugacy class of a parabolic subgroup of $\mathrm{GL}(V)$. Pick representatives $\widetilde{P}_i$ for these conjugacy classes, $i = 1, ..., b$, and define

$$\widetilde{\widetilde{\mathfrak{F}}}_i := \Big(\mathscr{I}\!som\big(V \otimes \mathscr{O}_{\mathfrak{Y}}, E_{\mathfrak{Y}|(\mathfrak{Y}\times\{x_i\})}\big)\Big)/\widetilde{P}_i, \quad i = 1, ..., b,$$

and

$$\mathfrak{F}_{\varrho\text{-FlPsBun}} := \widetilde{\widetilde{\mathfrak{F}}}_1 \times_{\mathfrak{Y}} \cdots \times_{\mathfrak{Y}} \widetilde{\widetilde{\mathfrak{F}}}_b.$$

Remark 5.7.2. Since the vector bundle $E_{\mathfrak{Y}}$ is linearized, $\widetilde{\widetilde{\mathfrak{F}}}_i$, $i = 1, ..., b$, and $\mathfrak{F}_{\varrho\text{-FlPsBun}}$ inherit $\mathrm{GL}(Y)$-actions. The equivalence relation on geometric points that is induced by the group action on $\mathfrak{F}_{\varrho\text{-FlPsBun}}$ is isomorphy of ϱ-flagged pseudo G-bundles.

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The Critical Values of Generalizations of the Hurwitz Zeta Function

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Abstract. We investigate a few types of generalizations of the Hurwitz zeta function, written $Z(s, a)$ in this abstract, where s is a complex variable and a is a parameter in the domain that depends on the type. In the easiest case we take $a \in \mathbf{R}$, and one of our main results is that $Z(-m, a)$ is a constant times $E_m(a)$ for $0 \leq m \in \mathbf{Z}$, where E_m is the generalized Euler polynomial of degree n. In another case, a is a positive definite real symmetric matrix of size n, and $Z(-m, a)$ for $0 \leq m \in \mathbf{Z}$ is a polynomial function of the entries of a of degree $\leq mn$. We will also define Z with a totally real number field as the base field, and will show that $Z(-m, a) \in \mathbf{Q}$ in a typical case.

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Introduction

This paper is divided into four parts. In the first part we consider a generalization of Hurwitz zeta function given by

$$\zeta(s;\, a,\, \gamma) = \sum_{n=0}^{\infty} \gamma^n (n+a)^{-s}, \tag{0.1}$$

where $s \in \mathbf{C}$, $0 < a \in \mathbf{R}$, and $\gamma \in \mathbf{C}$, $0 < |\gamma| \leq 1$. Clearly the infinite series is convergent for $\mathrm{Re}(s) > 1$. For $\gamma = 1$ this becomes $\sum_{n=0}^{\infty}(n+a)^{-s}$, which is the classical Hurwitz zeta function usually denoted by $\zeta(s, a)$. This generalization is not new. It was considered by Lerch in [Le], a work five years after the paper [Hu] of Hurwitz in 1882. Its analytic properties can be summarized as follows.

Theorem 0.1. *For a and γ as above the product $(e^{2\pi i s}-1)\Gamma(s)\zeta(s;\, a,\, \gamma)$ can be continued to an entire function in s. In addition, there exists a holomorphic function in $(s, a, \gamma) \in \mathbf{C}^3$, defined for $\mathrm{Re}(a) > 0$ and $\gamma \notin \{x \in \mathbf{R} \mid x \geq 1\}$ with no condition on s, that coincides with the product when $\mathrm{Re}(s) > 1$, $0 < a \in \mathbf{R}$, and $0 < |\gamma| \leq 1$.*

The proof will be given in §1.1.

To state a more interesting fact, we first put

$$\mathbf{e}(z) = \exp(2\pi i z) \qquad (z \in \mathbf{C}), \tag{0.2}$$

and define a function $E_{c,n}(t)$ in t for $c \in \mathbf{C}$ and $0 < n \in \mathbf{Z}$, that is called the *nth generalized Euler polynomial*, by

$$\frac{(1+c)e^{tz}}{e^z + c} = \sum_{n=0}^{\infty} \frac{E_{c,n}(t)}{n!} z^n. \tag{0.3}$$

We assume $c = -\mathbf{e}(\alpha)$ with $\alpha \in \mathbf{R}, \notin \mathbf{Z}$. The function $E_{c,n}(t)$ was introduced in [S07]. If $c = 1$, $E_{1,n}(t)$ is the classical Euler polynomial of degree n. In [S07] we showed that $E_{c,n}(t)$ is a polynomial in t of degree n; it is also a polynomial in $(1+c)^{-1}$. Its properties are listed in [S07, pp. 25–26]. We mention here only

$$E_{c,n}(1-t) = (-1)^n E_{c^{-1},n}(t), \tag{0.3a}$$

(see [S07, (4.3f)]), which will become necessary later. Now we have

THEOREM 0.2. *For $0 < k \in \mathbf{Z}$, $\mathrm{Re}(a) > 0$, and $\gamma \notin \{x \in \mathbf{R} \mid x \geq 1\}$ the value $\zeta(1-k,\, a;\, \gamma)$ is a polynomial function of a and $(\gamma - 1)^{-1}$. More precisely, we have*

$$\zeta(1-k;\, a,\, \gamma) = E_{c,k-1}(a)/(1 + c^{-1}) \tag{0.4}$$

for such k, a, and γ, where $c = -\gamma^{-1}$.

This will be proven in §1.2.

As for the original Hurwitz function, there is a well known relation

$$\zeta(1-k,\, a) = -B_k(a)/k \quad \text{for} \quad 0 < k \in \mathbf{Z}, \tag{0.5}$$

where B_k is the k-th Bernoulli polynomial. This is essentially due to Hurwitz; see [Hu, p. 92]; cf. also [E, p.27, (11)] and [WW, p. 267, 13.14].

In [S07] and [S08] we investigated the critical values of the L-function $L(s,\, \chi)$ with a Dirichlet character χ, and proved especially (see [S07, Theorem 4.14] and [S08, Theorem 1.4])

THEOREM 0.3. *Let χ be a nontrivial primitive Dirichlet character modulo a positive integer d, and let k be a positive integer such that $\chi(-1) = (-1)^k$.*

(i) *If $d = 2q + 1$ with $0 < q \in \mathbf{Z}$, then*

$$L(1-k,\, \chi) = \frac{d^{k-1}}{2^k \chi(2) - 1} \sum_{b=1}^{q} (-1)^b \chi(b) E_{1,k-1}(b/d). \tag{0.6}$$

(ii) *If $d = 4d_0$ with $1 < d_0 \in \mathbf{Z}$, then*

$$L(1-k,\, \chi) = (2d_0)^{k-1} \sum_{a=1}^{d_0 - 1} \chi(a) E_{1,k-1}(2a/d). \tag{0.7}$$

In §1.4 we will give a shorter proof for these formulas by means of (0.4), and in Section 2 we will prove a functional equation for $\zeta(s;\, a, \gamma)$ by producing an expression for $\zeta(1-s;\, a,\, \gamma)$.

The second part of the paper concerns the analogue of (0.1) defined when the base field is a totally real algebraic number field F. If $F \neq \mathbf{Q}$, there are nontrivial units, which cause considerable difficulties, and for this reason we cannot give a full generalization of which (0.1) is a special case. However, taking such an F as the base field, we will present a function of a complex variable s and two parameters a and p in F, that includes as a special case at least $\zeta(s;\, a,\, \gamma)$ with $a \in \mathbf{Q}$ and γ a root of unity. We then prove in Theorem 3.4 a rationality result on its critical values.

The third part is a kind of interlude. Observing that the formula for $L(k,\, \chi)$ (not $L(1-k,\, \chi)$) involves the Gauss sum $G(\chi)$ of χ, we will give in Section 4 a formula for $G(\chi\lambda)/G(\chi)$ for certain Dirichlet characters χ and λ.

The fourth and final part of the paper, which has a potential of future development, concerns the analogue of (0.1) defined for a complex variable s, with nonnegative and positive definite symmetric matrices of size n in place of n and a. We will show in Section 5 that it is an entire function of s and also that its value at $s = -m$ for $0 \le m \in \mathbf{Z}$ is a polynomial function of the variable symmetric matrix of degree $\le mn$.

1. Proof of Theorems 0.1, 0.2, and 0.3

1.1. To prove Theorem 0.1, assuming that $0 < a \in \mathbf{R}$ and $0 < |\gamma| \le 1$, we start from an easy equality $\Gamma(s)(n+a)^{-s} = \int_0^\infty x^{s-1}e^{-(n+a)x}dx$. Therefore

$$\Gamma(s)\zeta(s;\, a,\, \gamma) = \sum_{n=0}^{\infty} \Gamma(s)\gamma^n(n+a)^{-s} = \sum_{n=0}^{\infty}\int_0^\infty x^{s-1}\gamma^n e^{-(n+a)x}dx$$
$$= \int_0^\infty \sum_{n=0}^{\infty} x^{s-1}\gamma^n e^{-(n+a)x}dx = \int_0^\infty \frac{x^{s-1}e^{-ax}}{1-\gamma e^{-x}}dx.$$

Our calculation is justified for $\sigma = \mathrm{Re}(s) > 1$, since

$$\sum_{n=0}^{\infty}\int_0^\infty \left|x^{s-1}\gamma^n e^{-(n+a)x}\right|dx \le \sum_{n=0}^{\infty}\Gamma(\sigma)(n+a)^{-\sigma} < \infty.$$

Thus we obtain

$$\Gamma(s)\zeta(s;\, a,\, \gamma) = \int_0^\infty \frac{x^{s-1}e^{x(1-a)}}{e^x-\gamma}dx \quad \text{for} \quad \mathrm{Re}(s) > 1. \tag{1.1}$$

We now consider

$$\int_\infty^{0+} \frac{z^{s-1}e^{z(1-a)}}{e^z-\gamma}dz$$

with the standard symbol $\int_\infty^{0+}$ of contour integration. The integral is the sum of three integrals: $\int_\infty^\delta$, $\oint$ on the circle $|z| = \delta$, and $\int_\delta^\infty$, where $0 < \delta \in \mathbf{R}$; we naturally take the limit as δ tends to 0. We take $z^{s-1} = \exp\bigl((s-1)\log z\bigr)$ for the first integral $\int_\infty^\delta$ with $\log z \in \mathbf{R}$ for $0 < z \in \mathbf{R}$; for the evaluation of the other integrals we continue z^{s-1} analytically without passing through the positive real axis. Then the first and third integrals produce

$$(\mathbf{e}(s)-1)\int_\delta^\infty \frac{x^{s-1}e^{x(1-a)}}{e^x-\gamma}dx,$$

which is meaningful for every $s \in \mathbf{C}$ and every $(a,\, \gamma) \in \mathbf{C}^2$ such that

(1.1a) $$\mathrm{Re}(a) > 0 \quad \text{and} \quad \gamma \notin \{x \in \mathbf{R} \,|\, x > 1\}.$$

As for $\oint$, we first observe that given $\gamma \in \mathbf{C}$, we can find a small $\delta_0 \in \mathbf{R}$, > 0, such that $e^z \neq \gamma$ for $0 < |z| \leq \delta_0$, since the map $z \mapsto w = e^z$ sends the punctured disc $0 < |z| \leq \delta_0$ into a punctured disc $0 < |w-1| < \varepsilon$ that does not contain γ. (This is clearly so even for $\gamma = 1$.) Therefore $\oint$ is meaningful for every $s \in \mathbf{C}$ and sufficiently small δ in both cases $\gamma \neq 1$ and $\gamma = 1$; the integral is independent of δ because of Cauchy's theorem. Now put $z = \delta e^{i\theta}$ with δ such that $0 < \delta < \delta_0$ and $0 \leq \theta < 2\pi$. Then $z^{s-1} = \exp\{(s-1)(\log\delta + i\theta)\}$, and so for $s = \sigma + i\tau$ with real σ and τ, we have $|z^{s-1}| = \delta^{\sigma-1}|e^{-\theta\tau}| \leq \delta^{\sigma-1}e^{2\pi|\tau|}$. If $\gamma \neq 1$, we see that $\mathrm{Min}_{|z|\leq\delta_0}|e^z - \gamma| > 0$, and so $|e^{z(1-a)}/(e^z-\gamma)|$ is bounded for $|z| \leq \delta_0$. If $\gamma = 1$, the function $e^{z(1-a)}/(e^z-\gamma)$ is $1/z$ plus a holomorphic function at $z = 0$. Thus for $0 < \delta \leq \delta_0$ we see that $\left|\oint\right| \leq M\delta^\sigma$ if $\gamma \neq 1$ and $\left|\oint\right| \leq M\delta^{\sigma-1}$ if $\gamma = 1$ with a constant M that depends on a, γ, and δ_0, and so $\oint$ tends to 0 as $\delta \to 0$ if $\mathrm{Re}(s) > 1$, and we obtain

(1.2) $$(\mathbf{e}(s) - 1)\Gamma(s)\zeta(s;\, a,\, \gamma) = \int_\infty^{0+} \frac{z^{s-1}e^{z(1-a)}}{e^z - \gamma}\,dz$$

for $0 < |\gamma| \leq 1$, $0 < a \in \mathbf{R}$, and $\mathrm{Re}(s) > 1$. (If $\gamma \neq 1$, the condition $\mathrm{Re}(s) > 0$ instead of $\mathrm{Re}(s) > 1$ is sufficient.) Now the right-hand side of (1.2) is meaningful for every $(s, a, \gamma) \in \mathbf{C}^3$ under condition (1.1a) and so it establishes the product on the left-hand side as an entire function of s. If $\gamma \neq 1$, the contour integral can define the product for the variables s, a, γ as described in Theorem 0.1. The integrand as a function of (z, s, a, γ) is not finite in a domain including $\gamma = 1$, and so the result for $\gamma = 1$ must be stated separately.

Remark. If $0 < |\gamma| \leq 1$ and $\gamma \neq 1$, then the series of (0.1) is convergent for $\mathrm{Re}(s) > 0$ and defines a holomorphic function of s there. This is clear if $|\gamma| < 1$. For $|\gamma| = 1$ and $\gamma \neq 1$, this follows from [S07, Lemma 4.3].

We are interested in the value of $\zeta(s;\, a,\, \gamma)$ at $s = -m$ with $0 \leq m \in \mathbf{Z}$. We first note

$$\bigl\{(\mathbf{e}(s) - 1)\Gamma(s)\bigr\}_{s=-m} = 2\pi i(-1)^m/m!.$$

For $s = -m$ the function z^{s-1} in the integrand is a one-valued function, and so $\int_\infty^\delta + \int_\delta^\infty = 0$. Therefore

(1.3) $$\int_\infty^{0+} = \oint = 2\pi i \cdot \mathrm{Res}_{z=0}\, \frac{z^{-m-1}e^{(1-a)z}}{e^z - \gamma}.$$

By (0.3), for $\gamma \neq 1$ we have

$$\frac{z^{-m-1}e^{(1-a)z}}{e^z - \gamma} = \frac{1}{1-\gamma}\sum_{n=0}^\infty \frac{E_{-\gamma,n}(1-a)}{n!}z^{n-m-1},$$

and so the residue in question is $(1-\gamma)^{-1}E_{-\gamma,m}(1-a)/m!$. Combining this with (0.3a) and (1.2), we obtain

(1.4) $$\zeta(-m;\, a,\, \gamma) = E_{c,m}(a)/(1 + c^{-1}) \quad \text{for} \quad 0 \leq m \in \mathbf{Z},$$

where $c = -\gamma^{-1}$. This proves (0.4). In [S07, p. 26] we showed that $E_{c,\,n}(t)$ is a polynomial in t and $(1+c)^{-1}$. For $c = -\gamma^{-1}$ we have $(1+c)^{-1} = 1+(\gamma-1)^{-1}$, and so we obtain Theorem 0.2.

For the reader's convenience, we give a proof of (0.5) here. If $\gamma = 1$, instead of (0.2) we use $ze^{tz}/(e^z-1) = \sum_{n=0}^{\infty} B_n(t)z^n/n!$. Then we obtain (0.5) in the same manner as in the case $\gamma \neq 1$.

1.3. Let us insert here a historical remark. Fixing a positive integer m and an integer a such that $0 \le a \le m$, Hurwitz considered in [Hu] an infinite series

$$f(s,\,a) = \sum_{n=0}^{\infty}(mn+a)^{-s}. \tag{1.5}$$

Since this depends on m, he also denoted it by $f(s,\,a|m)$. He proved analytic continuation of these functions and stated a functional equation for $f(1-s,\,a)$, basically following Riemann's methods for the investigation of $\zeta(s)$ in [R]. At that time not much was known about Dirichlet's L-function beyond his formulas for the class number of a binary quadratic form and his theorem about prime numbers in an arithmetic progression. Employing the results on $f(s,\,a)$, Hurwitz was able to prove that the L-function for a quadratic character has analytic continuation and satisfies a functional equation. Using the standard notation $\zeta(s,\,a) = \sum_{n=0}^{\infty}(n+a)^{-s}$ employed at present, we have $f(s,\,a|m) = m^{-s}\zeta(s,\,a/m)$, and so he considered $\zeta(s,\,a)$ only for $a \in \mathbf{Q}$. It is noticeable however that he proved essentially (0.5) as we already said.

As noted at the beginning of the paper, Lerch investigated the series of (0.1); one can also find an exposition of this topic in [E, p. 27, §1.11]. The paper [Li] of Lipschitz may be mentioned in this connection.

1.4. Let the symbols be as in Theorem 0.3(i). Put

$$\Lambda(s) = \sum_{n=1}^{\infty}(-1)^n\chi(n)n^{-s}.$$

Then $\Lambda(s) + L(s,\,\chi) = 2\sum_{n=1}^{\infty}\chi(2n)(2n)^{-s} = \chi(2)2^{1-s}L(s,\,\chi)$, and so

$$\Lambda(s) = L(s,\chi)\big\{\chi(2)2^{1-s}-1\big\}. \tag{1.6}$$

Since $\big\{a\,\big|\,1 \le a < d\big\} = \big\{a\,\big|\,1 \le a \le q\big\} \sqcup \big\{d-a\,\big|\,1 \le a \le q\big\}$, we have

$$\Lambda(s) = \sum_{a=1}^{q}\sum_{n=0}^{\infty}(-1)^{nd+a}\chi(a)(nd+a)^{-s} + \sum_{a=1}^{q}\sum_{n=0}^{\infty}(-1)^{nd+d-a}\chi(-a)(nd+d-a)^{-s},$$

and so $d^s\Lambda(s)$ equals

$$\sum_{a=1}^{q}(-1)^a\chi(a)\bigg\{\sum_{n=0}^{\infty}(-1)^n\Big(n+\frac{a}{d}\Big)^{-s} - \chi(-1)\sum_{n=0}^{\infty}(-1)^n\Big(n+\frac{d-a}{d}\Big)^{-s}\bigg\}$$
$$= \sum_{a=1}^{q}(-1)^a\chi(a)\big\{\zeta(s;\,a/d,\,-1) - (-1)^k\zeta(s;\,1-a/d,\,-1)\big\}.$$

Putting $s = 1-k$ and employing (0.4) and (0.3a), we obtain (0.6).

Our next task is to prove (0.7). Let $d = 4d_0$ with $1 < d_0 \in \mathbf{Z}$ as in Theorem 1.3(ii). We note an easy fact(see [S08, Lemma 1.3]):

$$\chi(2d_0 + a) = -\chi(a) \quad \text{for every} \quad a \in \mathbf{Z}. \tag{1.7}$$

Observe that $\{x \in \mathbf{Z} \mid x > 0,\, d_0 \nmid x\}$ is a disjoint union

$$(*) \quad \{nd + a \mid 0 < a < d_0,\ 0 \le n \in \mathbf{Z}\} \sqcup \{nd + 2d_0 + a \mid 0 < a < d_0,\ 0 \le n \in \mathbf{Z}\}$$
$$\sqcup \{nd - a \mid 0 < a < d_0,\ 0 < n \in \mathbf{Z}\} \sqcup \{nd + 2d_0 - a \mid 0 < a < d_0,\ 0 \le n \in \mathbf{Z}\}.$$

The sum of $\sum \chi(x)x^{-s}$ for x belonging to the first two sets equals

$$\sum_{a=1}^{d_0-1}\left\{\sum_{\nu=0}^{\infty}\chi(a)(4\nu d_0 + a)^{-s} + \sum_{\nu=0}^{\infty}\chi(2d_0 + a)\big(2(2\nu+1)d_0 + a\big)^{-s}\right\}.$$

Employing (1.7), we see that this equals

$$\sum_{a=1}^{d_0-1}\sum_{m=1}^{\infty}(-1)^m\chi(a)(2md_0 + a)^{-s} = (2d_0)^{-s}\sum_{a=1}^{d_0-1}\chi(a)\zeta(s;\, 2a/d, -1). \tag{1.8}$$

Similarly, from the last two sets of $(*)$ we obtain

$$\sum_{a=1}^{d_0-1}\left\{\sum_{\nu=1}^{\infty}\chi(-a)(4\nu d_0 - a)^{-s} + \sum_{\nu=0}^{\infty}\chi(2d_0 - a)\big(2(2\nu+1)d_0 - a\big)^{-s}\right\}$$
$$= -\sum_{a=1}^{d_0-1}\sum_{m=0}^{\infty}\chi(-a)(-1)^m(2md_0 + 2d_0 - a)^{-s}$$
$$= -(2d_0)^{-s}\sum_{a=1}^{d_0-1}\chi(-a)\zeta(s;\, 1 - 2a/d,\, -1)$$

by (1.7). Thus, adding (1.8) to this and putting $s = 1-k$, from (0.4) we obtain

$$(2d_0)^{1-k}L(1-k,\, \chi) = 2^{-1}\sum_{a=1}^{d_0-1}\chi(a)\big\{E_{1,k-1}(2a/d) - \chi(-1)E_{1,k-1}(1-2a/d)\big\}.$$

Suppose $\chi(-1) = (-1)^k$; then applying (0.3a) to $E_{1,k-1}(1-2a/d)$, we obtain (0.7). The proof of Theorem 0.3 is now complete

1.5. The case $d = 4$ is excluded in Theorem 0.3(ii). In this case, however, the matter is simpler. Indeed, for $\mu_4(n) = \left(\dfrac{-1}{n}\right)$ we have

$$L(s,\, \mu_4) = \sum_{m=0}^{\infty}(-1)^m(2m+1)^{-s}$$
$$= 2^{-s}\sum_{m=0}^{\infty}(-1)^m(m+1/2)^{-s} = 2^{-s}\zeta(s;\, 1/2,\, -1),$$

and so by (0.4) we obtain

$$L(1-k,\, \mu_4) = 2^{k-2}E_{1,k-1}(1/2) = E_{1,k-1}/2 \tag{1.9}$$

for every odd positive integer k, where $E_{1,n}$ denotes the nth Euler number. This is classical, except that the result is usually given in terms of $L(k,\, \mu_4)$ instead of $L(1-k,\, \mu_4)$.

1.6. Let us now show that a special case of Theorem 0.3(ii) can be given in a somewhat different way. Let ψ be a primitive character whose conductor d is odd, μ_4 the primitive character modulo 4 as above, and k a positive integer such that $\psi(-1) = (-1)^{k+1}$; put $m = (d-1)/2$. Then

$$L(1-k,\, \psi\mu_4) = (-1)^m (2d)^{k-1} \sum_{j=1}^{m} (-1)^j \psi(2j) E_{1,k-1}\bigl(\tfrac{1}{2} + \tfrac{j}{d}\bigr). \tag{1.10}$$

This was given in [S07, (6.2)], if in terms of $L(k,\, \psi\mu_4)$, but we can derive it also from Theorem 0.3(ii) as follows. Take $\chi = \psi\mu_4$ in (0.7). Then the sum on the right-hand side of (0.7) is $\sum_{a=1}^{2m} \chi(a) E_{1,k-1}(a/2d)$, which equals $\sum_{b=1}^{2m} \chi(d-b) E_{1,k-1}\bigl((d-b)/2d\bigr)$. Since the bth term is nonvanishing only for even b, employing (0.3a), we see that the last sum equals $\psi(-1)$ times $\sum_{j=1}^{m} (\psi\mu_4)(d-2j) E_{1,k-1}\bigl((d+2j)/2d\bigr)$. Since $d - 2j = 2(m-j) + 1$, we have $\mu_4(d-2j) = (-1)^{m-j}$, and so we obtain (1.10).

1.7. We can show that $\zeta(-m;\, a,\, \gamma)$ for $0 \le m \in \mathbf{Z}$ is a polynomial in a by a formal calculation as follows. Assuming that $|\gamma| < 1$, we have

$$\zeta(-m;\, a,\, \gamma) = a^m + \sum_{n=1}^{\infty} \gamma^n (n+a)^m = a^m + \sum_{\nu=0}^{m} \binom{m}{\nu} a^{m-\nu} c_\nu$$

with $c_\nu = \sum_{n=1}^{\infty} n^\nu \gamma^n$, and so $\zeta(-m;\, a,\, \gamma)$ is a polynomial in a at least for $|\gamma| < 1$, and so Theorem 0.1 guarantees the same in a larger domain as described in that theorem

We have $c_{\nu-1} = \gamma(1-\gamma)^{-\nu} P_\nu(\gamma)$ for $1 \le \nu \in \mathbf{Z}$ with a polynomial P_ν introduced in [S07, (2.16)]; see also [S08, (4.3)]. We showed that $P_{\nu+1}(\gamma) = (\gamma - 1)^\nu E_{-\gamma,\nu}(0)$ for $\nu > 0$ in [S07, (4.6)] and that $\gamma^{n-2} P_n(\gamma^{-1}) = P_n(\gamma)$ in [S07, (2.19)]; also, $E_{c,n}(t) = \sum_{k=0}^{n} \binom{n}{k} E_{c,k}(0) t^{n-k}$ by [S08, (1.15)]. Combining these together, we obtain (0.4).

Though clearly this is not the best way to prove (0.4), at least it explains an elementary aspect of the nature of the problem. In Section 5, we will return to this idea in our discussion in the higher-dimensional case.

2. The functional equation for $\zeta(s;\, a,\, \gamma)$

2.1. For $\mathrm{Re}(s) > 1$ Hurwitz proved (see [Hu, p. 93, 1)] and [WW, p. 269])

$$\begin{aligned} \zeta(1-s,\, a) & \\ &= \frac{2\Gamma(s)}{(2\pi)^s} \left\{ \cos(\pi s/2) \sum_{n=1}^{\infty} \frac{\cos(2\pi na)}{n^s} + \sin(\pi s/2) \sum_{n=1}^{\infty} \frac{\sin(2\pi na)}{n^s} \right\}. \end{aligned} \tag{2.1}$$

Therefore it is natural to ask if there is a meaningful formula for $\zeta(1-s,\, a;\, \gamma)$. Though this was essentially done by Lerch in [Le], here we take a different approach. For $s \in \mathbf{C}$, $a \in \mathbf{R}$, $p \in \mathbf{R}$, and $\nu = 0$ or 1 we put

$$D^\nu(s;\, a,\, p) = \sum_{-a \ne n \in \mathbf{Z}} (n+a)^\nu |n+a|^{-\nu-s} \mathbf{e}\bigl(p(n+a)\bigr), \tag{2.2}$$

(2.3) $$T^\nu(s;\,a,\,p)=g_\nu(s)D^\nu(s;\,a,\,p),\quad g_\nu(s)=\pi^{-(s+\nu)/2}\Gamma\bigl((s+\nu)/2\bigr).$$

These were introduced in [S08]. In particular, we proved

(2.4) $$T^\nu(1-s;\,a,\,p)=i^{-\nu}\mathbf{e}(ap)T^\nu(s;\,-p,\,a).$$

Let $\gamma=\mathbf{e}(p)$ and $b=1-a$ with $0<a<1$. Then it is easy to verify that

(2.5a) $$D^0(s;\,a,\,p)=\mathbf{e}(ap)\zeta(s;\,a,\,\gamma)+\mathbf{e}(-bp)\zeta(s;\,b,\,\gamma^{-1}),$$

(2.5b) $$D^1(s;\,a,\,p)=\mathbf{e}(ap)\zeta(s;\,a,\,\gamma)-\mathbf{e}(-bp)\zeta(s;\,b,\,\gamma^{-1}),$$

and so

(2.6) $$2\mathbf{e}(ap)\zeta(s;\,a,\,\gamma)=D^0(s;\,a,\,p)+D^1(s;\,a,\,p).$$

Employing (2.3) and (2.4), we obtain

(2.7) $$2\zeta(1-s;\,a,\,\gamma)=\frac{g_0(s)}{g_0(1-s)}D^0(s;\,-p,\,a)-\frac{ig_1(s)}{g_1(1-s)}D^1(s;\,-p,\,a).$$

From (2.5a, b) we see that $D^\nu(s;\,-p,\,a)$ is a linear combination of $\zeta(s;\,-p,\,\delta)$ and $\zeta(s;\,1+p,\,\delta^{-1})$, where $\delta=\mathbf{e}(a)$. Thus, for $-1<p<0$ we have

$$2\zeta(1-s;\,a,\,\gamma)=\mathbf{e}(-ap)A\zeta(s;\,-p,\,\delta)+\mathbf{e}(-a-ap)B\zeta(s;\,1+p,\,\delta^{-1})$$

with

(2.8) $$A=\frac{g_0(s)}{g_0(1-s)}-\frac{ig_1(s)}{g_1(1-s)},\qquad B=\frac{g_0(s)}{g_0(1-s)}+\frac{ig_1(s)}{g_1(1-s)}.$$

Recalling that $\Gamma(s/2)\Gamma((s+1)/2)=2^{1-s}\pi^{1/2}\Gamma(s)$ and $\Gamma(s)\Gamma(1-s)=\pi/\sin(\pi s)$, we find that

(2.9) $$A=2^{1-s}\pi^{-s}\mathbf{e}(-s/4)\Gamma(s),\qquad B=2^{1-s}\pi^{-s}\mathbf{e}(s/4)\Gamma(s),$$

and so we obtain

(2.10) $$\zeta(1-s;\,a,\,\gamma)=\frac{\mathbf{e}(-ap)\Gamma(s)}{(2\pi)^s}\Bigl\{\mathbf{e}(-s/4)\zeta(s;\,-p,\,\delta)+\mathbf{e}(s/4-a)\zeta(s;\,p+1,\,\delta^{-1})\Bigr\}.$$

at least when $-1<p<0$ and $0<a<1$, where $\gamma=\mathbf{e}(p)$ and $\delta=\mathbf{e}(a)$.

This does not apply to the case $\gamma=1$. In this case we have

$$2\zeta(s;\,a,\,1)=D^0(s;\,a,\,0)+D^1(s;\,a,\,0)\quad\text{for}\quad 0<a\le 1,$$
$$D^\nu(s;\,0,\,a)=\delta\zeta(s;\,1,\,\delta)+(-1)^\nu\delta^{-1}\zeta(s;\,1,\,\delta^{-1}).$$

Repeating the same argument as in the case $\gamma\ne 1$, we find that

$$2\zeta(1-s;\,a,\,1)=\delta A\zeta(s;\,1,\,\delta)+\delta^{-1}B\zeta(s;\,1,\,\delta^{-1})$$

with the same A and B as in (2.8) and (2.9), and so

(2.11) $$\zeta(1-s;\,a,\,1)=\frac{\Gamma(s)}{(2\pi)^s}\Bigl\{\mathbf{e}\Bigl(a-\frac{s}{4}\Bigr)\zeta(s;\,1,\,\delta)+\mathbf{e}\Bigl(\frac{s}{4}-a\Bigr)\zeta(s;\,1,\,\delta^{-1})\Bigr\}.$$

where $\delta=\mathbf{e}(a)$, $0<a\le 1$. This gives (2.1). Indeed, we have

$$\mathbf{e}(\pm a)\zeta(s;\,1,\,\delta^{\pm 1}) = \sum_{m=1}^{\infty}\frac{\delta^{\pm m}}{m^s} = \sum_{m=1}^{\infty}\frac{\cos(2\pi ma) \pm i\sin(2\pi ma)}{m^s},$$

and so a simple calculation transforms (2.11) into (2.1).

Returning to (2.10) in which we assumed $-1 < p < 0$, put $q = -p$. Then $0 < q < 1$ and

$$\begin{aligned}(2.12)\qquad &\frac{(2\pi)^s}{\Gamma(s)}\zeta\bigl(1-s;\,a,\,\mathbf{e}(q)^{-1}\bigr)\\ &= \mathbf{e}(-s/4)\sum_{h=0}^{\infty}\frac{\mathbf{e}\bigl(a(h+q)\bigr)}{(h+q)^s} + \mathbf{e}(s/4)\sum_{h=0}^{\infty}\frac{\mathbf{e}\bigl(a(q-h-1)\bigr)}{(h+1-q)^s}.\end{aligned}$$

Then employing (0.4), for $0 < s = k \in \mathbf{Z}$ we obtain

$$(2.13)\qquad \frac{(2\pi i)^k}{(k-1)!(1+c^{-1})}E_{c,k-1}(a) = \sum_{h\in\mathbf{Z}}\frac{\mathbf{e}\bigl(a(h+q)\bigr)}{(h+q)^k},$$

where $c = -\mathbf{e}(q)$. This formula was given in [S07, (4.5)]. Thus we have given a proof of (2.13) different from that of [S07]. (The case $k = 1$ must be handled carefully; see [S07, pp. 26–27].) In [S08] we asked the question whether the parameter k in (2.13) can be extended to a complex variable, and presented $D^{\nu}(s;\,a,\,p)$ as an answer. Since (2.13) is a special case of (2.12), we can now say that (2.12) is another answer to that question.

3. The case of a totally real number field

3.1. Let F be a totally real algebraic number field. We ask whether we can define a function similar to $\zeta(s;\,a,\,\gamma)$ by taking the totally positive integers in F in place of n in (0.1). We are going to give a partially affirmative answer to this question. We let $\mathfrak{g}$ denote the maximal order of F, $\mathfrak{d}$ the different of F relative to $\mathbf{Q}$, and $\mathbf{a}$ the set of all archimedean primes of F. For each $v \in \mathbf{a}$ we denote by F_v the v-completion of F, identified with $\mathbf{R}$. In other words, v defines an injection of F into $\mathbf{R}$, and for $\xi \in F$ we denote by ξ_v the image of ξ under this injection. We put $[F:\mathbf{Q}] = g$, $F_{\mathbf{a}} = \prod_{v\in\mathbf{a}} F_v$, and $F_{\mathbf{a}}^{\times} = \prod_{v\in\mathbf{a}} F_v^{\times}$. Then $F_{\mathbf{a}}$ can be identified with $\mathbf{R}^g$, and for $\xi \in F$ the map $\xi \mapsto (\xi_v)_{v\in\mathbf{a}}$ defines an injection of F into $F_{\mathbf{a}}$. We then put

$$\mathbf{e}_{\mathbf{a}}(\xi) = \mathbf{e}\bigl(\textstyle\sum_{v\in\mathbf{a}}\xi_v\bigr) \qquad (\xi \in F_{\mathbf{a}}),$$

$$\xi^k = \prod_{v\in\mathbf{a}}\xi_v^{k_v}, \qquad \xi^{\mathbf{a}} = \prod_{v\in\mathbf{a}}\xi_v, \qquad (k = (k_v)_{v\in\mathbf{a}} \in \mathbf{Z}^{\mathbf{a}},\ \xi \in F_{\mathbf{a}}^{\times}).$$

We also put $N(\xi) = N_{F/\mathbf{Q}}(\xi)$ for $\xi \in F$. Then $N(\xi\mathfrak{g}) = |N(\xi)| = |\xi^{\mathbf{a}}|$ for $\xi \in F^{\times}$. We write $\xi \gg 0$ if $\xi_v > 0$ for every $v \in \mathbf{a}$ and put $\mathfrak{g}_+^{\times} = \bigl\{u \in \mathfrak{g}^{\times} \bigm| u \gg 0\bigr\}$.

Now for $s \in \mathbf{C}$, a fractional ideal $\mathfrak{b}$, and $a,\, p \in F$ we put

$$(3.1)\qquad \zeta(s;\,\mathfrak{b},\,a,\,p) = [\mathfrak{g}_+^{\times} : U]^{-1}\sum_{0\ll\xi\in\mathfrak{b}+a \pmod{U}}|N(\xi)|^{-s}\mathbf{e}_{\mathbf{a}}(p\xi).$$

Here the sum is taken over $F^{\times}/U$ under the condition that $\xi \gg 0$ and $\xi - a \in \mathfrak{b}$. We take a subgroup U of $\mathfrak{g}_+^{\times}$ of finite index such that $u - 1 \in a^{-1}\mathfrak{b} \cap$

$p^{-1}(\mathfrak{b}^{-1}\mathfrak{d}^{-1} \cap a^{-1}\mathfrak{d}^{-1})$ for every $u \in U$. Clearly such a U exists, the sum of (3.1) is meaningful, and $\zeta(s;\, \mathfrak{b},\, a,\, p)$ is well defined independently of the choice of U.

This is an analogue of (0.1), but it should be remembered that here both a and p belong to F. Thus (1.5) is a special case of (3.1).

Next, let $k \in \mathbf{Z}^{\mathbf{a}}$. With s, $\mathfrak{b}$, a, and p as above, we put

$$D_k(s;\, \mathfrak{b},\, a,\, p) = [\mathfrak{g}_+^\times : U]^{-1} \sum_{0 \neq \xi \in \mathfrak{b}+a \pmod{U}} \xi^{-k}|\xi|^{k-s\mathbf{a}}\mathbf{e}_{\mathbf{a}}(p\xi), \tag{3.2}$$

where the summation is the same as in (3.1) except that this time we do not impose the condition $\xi \gg 0$. This is well defined and both (3.1) and (3.2) are convergent for $\mathrm{Re}(s) > 1$.

Lemma 3.2. *Let $k \in \mathbf{Z}^{\mathbf{a}}$ with $k_v = 0$ or 1 for every $v \in \mathbf{a}$. Then the product*

$$D_k(s;\, \mathfrak{b},\, a,\, p)\prod_{v\in\mathbf{a}} \Gamma\big((s+k_v)/2\big)$$

can be continued to a meromorphic function of s on the whole s-plane that is holomorphic except for possible simple poles at $s = 0$ and 1, which occur only when $k = 0$. The pole at $s = 0$ occurs if and only if $k = 0$ and $a \in \mathfrak{b}$.

This is included in [S00, Lemma 18.2], as $D_k(s;\, \mathfrak{b},\, a,\, p)$ is a special case of the series $D_k(s,\, \kappa)$ of [S00, (18.1)]. Notice that $D_k(s;\, \mathfrak{b},\, a,\, p)$ is finite at $s = 0$ for every k.

Lemma 3.3. *For $0 < \mu \in \mathbf{Z}$ and $k \in \mathbf{Z}^{\mathbf{a}}$ with $k_v = 0$ or 1 the following assertions hold:*

(i) *$D_k(1-\mu;\, \mathfrak{b},\, a,\, p) = 0$ if $k_v - \mu \notin 2\mathbf{Z}$ for some $v \in \mathbf{a}$.*

(ii) *Suppose $k_v - \mu \in 2\mathbf{Z}$ for every $v \in \mathbf{a}$; then $D_k(1-\mu;\, \mathfrak{b},\, a,\, p) \in \mathbf{Q}_{\mathrm{ab}}$, where $\mathbf{Q}_{\mathrm{ab}}$ denotes the maximal abelian extension of $\mathbf{Q}$; in particular, $D_k(1-\mu;\, \mathfrak{b},\, a,\, 0) \in \mathbf{Q}$.*

Proof. Suppose $k_v - \mu \notin 2\mathbf{Z}$ for one particular v. Then $\Gamma\big((s+k_v)/2\big)$ has a pole at $s = 1-\mu$, and so (i) follows from Lemma 3.2. As for (ii), that $D_k(1-\mu;\, \mathfrak{b},\, a,\, 0) \in \mathbf{Q}$ is given in Proposition 18.10(ii) of [S00]. For any $p \in F$, we see that $D_k(s;\, \mathfrak{b},\, a,\, p)$ is a finite $\mathbf{Q}_{\mathrm{ab}}$-linear combination of $D_k(s;\, \mathfrak{b}',\, a',\, 0)$ with several $(\mathfrak{b}',\, a')$, and so $D_k(1-\mu;\, \mathfrak{b},\, a,\, p) \in \mathbf{Q}_{\mathrm{ab}}$.

Now our principal result on $\zeta(s;\, \mathfrak{b},\, a,\, p)$ can be stated as follows.

Theorem 3.4. (i) *$\zeta(s;\, \mathfrak{b},\, a,\, p)$ can be continued to a meromorphic function of s on the whole s-plane, which is holomorphic except for a possible simple pole at $s = 1$.*

(ii) *Let $0 < \mu \in \mathbf{Z}$. Then $\zeta(1-\mu;\, \mathfrak{b},\, a,\, p) \in \mathbf{Q}_{\mathrm{ab}}$, and in particular, $\zeta(1-\mu;\, \mathfrak{b},\, a,\, 0) \in \mathbf{Q}$.*

Proof. For $\xi \in F^\times$ we note an easy fact

$$\sum_{k\in\mathbf{Z}^{\mathbf{a}}/2\mathbf{Z}^{\mathbf{a}}} \xi^{-k}|\xi|^k = \begin{cases} 2^g & \text{if } \ \xi \gg 0, \\ 0 & \text{otherwise,} \end{cases}$$

where $g = [F : \mathbf{Q}]$. Therefore we obtain

$$2^g\zeta(s;\,\mathfrak{b},\,a,\,p)=\sum_{k\in\mathbf{Z}^{\mathbf{a}}/2\mathbf{Z}^{\mathbf{a}}}D_k(s;\,\mathfrak{b},\,a,\,p),\tag{3.3}$$

and so assertion (i) follows immediately from Lemma 3.2. Take μ as in (ii). By Lemma 3.3(i), the terms on the right-hand side of (3.3) vanish except for the term with k such that $k_v-\mu\in 2\mathbf{Z}$ for every v. Therefore we obtain the desired result from Lemma 3.3(ii), and our proof is complete.

4. Some explicit expressions for Gauss sums

4.1. There are two kinds of formulas for the critical values of $L(s,\,\chi)$: one is for $L(k,\,\chi)$ and the other for $L(1-k,\,\chi)$. The former involves π and the Gauss sum of χ, whereas the latter does not. In a sense $L(1-k,\,\chi)$ is conceptually more natural than $L(k,\,\chi)$, but there is an interesting aspect in the computation of $L(k,\,\chi)$, since it allows us to find an explicit expression for a certain Gauss sum. This can be achieved by computing $L(k,\,\chi)$ in two different ways, which involve two *different* Gauss sums. Let us begin with the definition of a Gauss sum and an easy lemma.

Given a primitive or an imprimitive Dirichlet character χ' modulo a positive integer, we take the primitive character χ associated with χ', and define the Gauss sum $G(\chi')$ to be the same as the Gauss sum $G(\chi)$ of χ, given by

$$G(\chi)=\sum_{a=1}^{d}\chi(a)\mathbf{e}(a/d),\tag{4.1}$$

where d is the conductor of χ. Now we have an elementary

Lemma 4.2. (i) *Let $\chi_1,\,\ldots\,,\chi_m$ be Dirichlet characters. Then the number $G(\chi_1)\cdots G(\chi_m)/G(\chi_1\cdots\chi_m)$ belongs to the field generated by the values of $\chi_1,\,\ldots\,,\chi_m$ over $\mathbf{Q}$.*

(ii) *Let ψ and χ be primitive characters of conductor c and d, respectively. If c and d are relatively prime, then*

$$G(\psi\chi)=\psi(d)\chi(c)G(\psi)G(\chi).\tag{4.2}$$

Proof. For the proof of (i) see [S78, Proposition 4.12], which generalizes [S76, Lemma 8]. In the setting of (ii) take $r,\,s\in\mathbf{Z}$ so that $cr+ds=1$. Then for $x,\,y\in\mathbf{Z}$ the map $(x,\,y)\mapsto xds+ycr$ gives a bijection of $(\mathbf{Z}/c\mathbf{Z})\times(\mathbf{Z}/d\mathbf{Z})$ onto $\mathbf{Z}/cd\mathbf{Z}$, and so

$$\begin{aligned}G(\psi\chi)&=\sum_{x=1}^{c}\sum_{y=1}^{d}\mathbf{e}\big((xds+ycr)/cd\big)\psi(xds)\chi(ycr)\\&=\sum_{x=1}^{c}\psi(xds)\mathbf{e}(xs/c)\sum_{y=1}^{d}\chi(ycr)\mathbf{e}(yr/d),\end{aligned}$$

which proves (4.2).

Theorem 4.3. *Let χ be a primitive character of conductor d such that $\chi(-1)=-1$, and let $\lambda(m)=\left(\frac{3}{m}\right)$. Suppose d is odd and $0<d/9\in\mathbf{Z}$. Then*

$$\frac{G(\chi\lambda)}{G(\chi)} = \left\{2\sqrt{3}\chi(2)\sum_{a=1}^{d-1}(\chi\lambda)(a)\right\}\Big/\left\{\sum_{j=1-g}^{d-g}(-1)^j\chi(j)\right\}, \tag{4.3}$$

where $g = [d/6] + 1$.

Proof. In [S07, Theorem 6.3(v)] we gave a formula for $L(k,\, \chi\lambda)$. Taking $k = 1$ and $\bar{\chi}$ in place of χ, we obtain

$$2\sqrt{3}\chi(2)(\pi i)^{-1}G(\chi)L(1,\, \bar{\chi}\lambda) = \sum_{j=1-g}^{d-g}(-1)^j\chi(j),$$

since $E_{1,0}(t) = 1$. Now $\bar{\chi}\lambda$ is primitive and has conductor $4d$, and so the formula [S07, (4.34)] applied to $\bar{\chi}\lambda$ produces

$$(\pi i)^{-1}G(\chi\lambda)L(1,\, \bar{\chi}\lambda) = \sum_{a=1}^{d-1}(\chi\lambda)(a).$$

Taking the quotient of these two formulas, we obtain (4.3).

In [S07, Theorem 6.3] we gave eight formulas for $L(k,\, \chi\lambda)$, where λ is a "constant" character and χ is a "variable" character. In the above theorem we employed only one of those formulas. We can actually state results about $G(\chi\lambda)/G(\chi)$ in the other seven cases, but they are not so interesting, since we can apply (4.2) to $\chi\lambda$ in those cases, and the case we employed in the above theorem is the only case to which (4.2) is not applicable. Even in that case, the significance of (4.3) is rather obscure. Still, the formula is clear-cut and nontrivial, and we state it here with the hope that future researchers will be able to clarify its nature in a better perspective.

We end our discussion of this subject by showing the quantity of (4.3) can be determined in a different way. We begin with some preliminary results.

Lemma 4.4. *Let χ and ψ be primitive characters of conductor p^m and p^n, respectively, where p is a prime number and m, n are positive integers. Suppose $m \geq n$ and $\chi\psi$ has conductor p^m. Then*

$$G(\chi)G(\psi) = G(\chi\psi)\sum_{a=1}^{p^n}\chi(1 - p^{m-n}a)\psi(a). \tag{4.4}$$

This was given in [S76, (4.2)].

Lemma 4.5. *Let χ be a primitive character of conductor c, where $c = 3^m$ with $m > 1$ or $c = 2^m$ with $m > 3$, and let μ_3 and μ_4 denote the primitive characters of conductor 3 and 4, respectively. Let $\chi' = \chi\mu_3$ if $c = 3^m$ and $\chi' = \chi\mu_4$ if $c = 2^m$. Then $G(\chi') = \varepsilon G(\chi)$ with $\varepsilon = \pm 1$ determined by $\chi(1 - 3^{m-1}) = \mathbf{e}(\varepsilon/3)$ if $c = 3^m$ and $\chi(1 - 2^{m-2}) = \mathbf{e}(\varepsilon/4)$ if $c = 2^m$.*

Proof. We first consider the case $c = 2^m$. By (4.4), $G(\chi)G(\mu_4)/G(\chi') = \beta - \gamma$ with $\beta = \chi(1-2^{m-2})$ and $\gamma = \chi(1+2^{m-2})$. Since $m > 3$, we have $(1-2^{m-2})^2 \equiv 1-2^{m-1} \pmod{2^m}$, $(1-2^{m-2})(1+2^{m-2}) \equiv 1 \pmod{2^m}$, and $(1-2^{m-2})^4 \equiv 1 \pmod{2^m}$, and so $\beta^4 = \beta\gamma = 1$. Suppose $\beta = \pm 1$. Then $\chi(1-2^{m-1}) = 1$, and so $\chi(1 - 2^{m-1}a) = \chi(1 - 2^{m-1})^a = 1$ for every $a \in \mathbf{Z}$, which means that χ

has conductor $\le 2^{m-1}$, a contradiction. Thus $\beta \neq \pm 1$, and so $\beta = \varepsilon i$ with $\varepsilon = \pm 1$. Since $G(\mu_4) = 2i$, we have $G(\chi)/G(\chi') = (\beta - \beta^{-1})/2i = \varepsilon$, which proves the case $c = 2^m$.

If $c = 3^m$, we have similarly $G(\chi)G(\mu_3)/G(\chi') = \beta - \gamma$ with $\beta = \chi(1-3^{m-1})$ and $\gamma = \chi(1+3^{m-1})$. We easily see that $\beta\gamma = \beta^3 = 1$ and $\beta \neq 1$. Since $G(\mu_3) = \sqrt{3}i$, we have $G(\chi)/G(\chi') = (\beta - \beta^{-1})/\sqrt{3}i = \varepsilon$, and ε is determined by $\beta = \mathbf{e}(\varepsilon/3)$. This completes the proof.

4.6. Returning to the setting of Theorem 4.3, put $d = 3^m f$ with $m \in \mathbf{Z}$ and $0 < f \in \mathbf{Z}$, $3 \nmid f$; put also $\chi = \chi_0\chi_1$ with characters χ_0 and χ_1 of conductor 3^m and f, respectively. Since $\lambda = \mu_3\mu_4$, we have $\chi\lambda = \chi_0\mu_3\chi_1\mu_4$. By (4.2) we have $G(\chi_1\mu_4) = 2i\chi_1(4)\mu_4(f)G(\chi_1)$, and so

$$\begin{aligned} G(\chi\lambda) &= (\chi_1\mu_4)(3^m)(\chi_0\mu_3)(4f)G(\chi_0\mu_3)G(\chi_1\mu_4) \\ &= 2i(-1)^m\chi_0(f)\chi(4)\chi_1(3^m)\lambda(f)G(\chi_0\mu_3)G(\chi_1). \end{aligned}$$

Also, $G(\chi) = \chi_0(f)\chi_1(3^m)G(\chi_0)G(\chi_1)$. Therefore

$$G(\chi\lambda)/G(\chi) = 2i(-1)^m\lambda(f)\chi(4)G(\chi_0\mu_3)/G(\chi_0).$$

Applying Lemma 4.5 to $G(\chi_0\mu_3)/G(\chi_0)$, we thus obtain

$$G(\chi\lambda)/G(\chi) = 2i(-1)^m\lambda(f)\chi(4)\varepsilon, \tag{4.5}$$

where $\varepsilon = \pm 1$ is determined by $\chi_0(1-3^{m-1}) = \mathbf{e}(\varepsilon/3)$.

5. The case of a domain of positivity

5.1. There is a natural analogue of $\zeta(s;\, a,\, \gamma)$ defined on the space of symmetric matrices. To be explicit, with a positive integer n we denote by V the set of all real symmetric matrices of size n, and write $h > 0$ resp. $h \ge 0$ for $h \in V$ when h is positive definite resp. nonnegative. We put $V_{\mathbf{C}} = V \otimes_{\mathbf{R}} \mathbf{C}$,

$$\kappa = (n+1)/2, \quad P = \{h \in V \mid h > 0\}, \quad \text{and}$$
$$\mathfrak{H} = \{x + iy \in V_{\mathbf{C}} \mid x \in V,\, y \in P\}.$$

For $h \in V$ we denote by $\lambda(h)$ and $\mu(h)$ the maximum and minimum absolute value of eigenvalues of h, respectively. We easily see that V is a normed space with $\lambda(h)$ as the norm of h, that is, $\lambda(ch) = |c|\lambda(h)$ for $c \in \mathbf{R}$ and $\lambda(h+k) \le \lambda(h) + \lambda(k)$. For $0 \le d \in \mathbf{Z}$ we denote by S_d the space of all $\mathbf{C}$-valued homogeneous polynomial functions on V of degree d. Here are two easy facts:

(5.1) $\quad \mathrm{tr}(gh) \ge \lambda(h)\mu(g) \quad$ if $\quad g,\, h \in P$.

(5.2) $|\xi(h)| \le c_\xi\lambda(h)^d$ for every $\xi \in S_d$ and $h \in V$ with a positive constant c_ξ that depends only on ξ.

To prove (5.1), we may assume that g is diagonal. For $g = \mathrm{diag}[\mu_1, \ldots, \mu_n]$ we have $\mathrm{tr}(gh) = \sum_{i=1}^n \mu_i h_{ii} \ge \mu(g)\mathrm{tr}(h) \ge \mu(g)\lambda(h)$, since $\mathrm{tr}(h)$ is the sum of all eigenvalues of h. As for (5.2), given $h \in V$, take an orthogonal matrix p so that $h = {}^t p \cdot \mathrm{diag}[\kappa_1, \ldots, \kappa_n]p$ with $\kappa_i \in \mathbf{R}$. Since $|p_{ij}| \le 1$ and $|\kappa_i| \le \lambda(h)$, we see that $|h_{ij}| \le n\lambda(h)$, from which we obtain (5.2).

We now consider three types of infinite series:

$$\Phi(s;\, L,\, a,\, z) = \sum_{h \in L} \det\big(2\pi i(h-z)\big)^{-s}\mathbf{e}\big(\mathrm{tr}(a(h-z))\big), \tag{5.3}$$

$$F(s;\, L,\, a,\, z) = \sum_{h\in L,\, h+a>0} \det(h+a)^{-s}\mathbf{e}\big(\mathrm{tr}(hz)\big), \tag{5.4}$$

$$F_0(s;\, L,\, a,\, z) = \sum_{0\le h\in L} \det(h+a)^{-s}\mathbf{e}\big(\mathrm{tr}(hz)\big). \tag{5.5}$$

Here $s \in \mathbf{C}$, L is a lattice in V, $a \in V$, $z \in \mathfrak{H}$, and the sum of (5.4) is extended over all $h \in L$ such that $h + a \in P$; the sum of (5.3) is simply over all $h \in L$; in (5.5) we assume that $a > 0$ and the sum is extended over all nonnegative h in L. For $z \in \mathfrak{H}$ and $s \in \mathbf{C}$ we define $\det(-2\pi iz)^s$ so that it coincides with $\det(2\pi p)^s$ if $z = ip$ with $p \in P$.

LEMMA 5.2. *For every $\xi \in S_d$ the infinite series*

$$\sum_{h\in L,\, h+a>0} \det(h+a)^s\xi(h+a)\mathbf{e}\big(\mathrm{tr}(hz)\big) \tag{5.6}$$

converges absolutely and locally uniformly for $(s,\, a,\, z) \in \mathbf{C}\times V\times\mathfrak{H}$.

Proof. For a fixed positive number α the number of $h \in L$ such that $\lambda(h)\le\alpha$ is finite, as $\{h\in V \,|\, \lambda(h)\le\alpha\}$ is compact and L is discrete in V. Thus, to prove the convergence of (5.6), we can restrict h to those that satisfy $\lambda(h) > \lambda(a)+1$ for every $a \in A$, where A is a fixed compact subset of V. For such an h we have $1 \le \lambda(h+a) < 2\lambda(h)$ and $\det(h+a) \le \lambda(h+a)^n \le 2^n\lambda(h)^n$. Also, by (5.2), $|\xi(h+a)| \le c_\xi\lambda(h+a)^d \le c_\xi 2^d\lambda(h)^d$. Thus for $\mathrm{Re}(s) = \sigma$ we have $|\det(h+a)^s\xi(h+a)| \le 2^{n\sigma+d}c_\xi\lambda(h)^{n\sigma+d}$. On the other hand, for $0 < N \in \mathbf{Z}$ the number of $h \in L$ such that $N \le \lambda(h) < N+1$ is less than CN^b with positive constants C and b. Put $g = 2\pi\mathrm{Im}(z)$. Then $|\mathbf{e}(\mathrm{tr}(hz))| = e^{-\mathrm{tr}(gh)}$. Since $-\mathrm{tr}(gh) \le -\lambda(h)\mu(g)$ by (5.1), our partial sum can be majorized by $2^{n\sigma+d}c_\xi C\sum_{N=1}^{\infty}(N+1)^{n\sigma+d+b}e^{-N\mu(g)}$, which proves our lemma.

THEOREM 5.3. (i) *The infinite series of (5.3)* converges absolutely and locally uniformly in $(s,\, a,\, z) \in \{s \in \mathbf{C} \,|\, \mathrm{Re}(s) > n\} \times V \times \mathfrak{H}$. Thus it defines a holomorphic function in s for $\mathrm{Re}(s) > n$.

(ii) *The infinite series of (5.4)* and *(5.5) converge absolutely and locally uniformly in $(s,\, a,\, z) \in \mathbf{C}\times V\times\mathfrak{H}$, and so they define entire functions of s.*

(iii) *For* $\mathrm{Re}(s) > n$ *we have*

$$\mathrm{vol}(V/L)F(\kappa - s;\, L,\, a,\, z) = \Gamma_n(s)\Phi(s;\, L',\, a,\, z), \tag{5.7}$$

where $L' = \{x \in V \,|\, \mathrm{tr}(xL) \subset \mathbf{Z}\}$ and

$$\Gamma_n(s) = \pi^{n(n-1)/4}\prod_{k=0}^{n-1}\Gamma\big(s-(k/2)\big).$$

(iv) *For* $0 \le m \in \mathbf{Z}$ *the values* $F(-m;\, L,\, a,\, z)$, $F_0(-m;\, L,\, a,\, z)$, *and* $\Phi(\kappa+m;\, L,\, a,\, z)$ *are polynomial functions of* a *of degree* $\le mn$, *whose coefficients depend on* L *and* z.

Statement (iv) for F_0 can be taken literally, but the cases of F and Φ require some clarifications, which will be given in the proof.

Proof. Assertion (i) is included in [S82, Lemma 1.3]; (ii) follows from Lemma 5.2. To prove (iii), given $s \in \mathbf{C}$ and $p \in P$, we consider a function g on V defined by

$$g(u) = \begin{cases} e^{-\mathrm{tr}(up)} \det(u)^{s-\kappa} & (u \in P), \\ 0 & (u \notin P), \end{cases}$$

and define its Fourier transform $\hat{g}$ by

$$\hat{g}(t) = \int_V \mathbf{e}\big(-\mathrm{tr}(ut)\big) g(u)du \qquad (t \in V),$$

where $du = \prod_{i \le j} du_{ij}$. As shown in [S82, (1.22)], $\hat{g}(t) = \Gamma_n(s)\det(p+2\pi i t)^{-s}$, provided $\mathrm{Re}(s) > \kappa - 1$. Then the Poisson summation formula establishes equality (5.7) with both sides multiplied by $\mathbf{e}\big(\mathrm{tr}(az)\big)$ for $z = (-2\pi i)^{-1}p$ when the series of (5.3) and (5.4) are convergent, which is the case at least when $\mathrm{Re}(s) > n$. Since both sides of (5.7) are holomorphic in z if $\mathrm{Re}(s) > n$, we obtain (iii) as stated.

To prove (iv), take a $\mathbf{C}$-basis B of $\sum_{d=0}^{mn} S_d$. For $0 \le m \in \mathbf{Z}$ we have

$$F_0(-m;\, L,\, a,\, z) = \sum_{0 \le h \in L} \det(h+a)^m \mathbf{e}\big(\mathrm{tr}(hz)\big). \tag{5.8}$$

We can put $\det(h+a)^m = \sum_{\beta \in B} \beta(a) f_\beta(h)$ with polynomial functions f_β, and so

$$F_0(-m;\, L,\, a,\, z) = \sum_{\beta \in B} \beta(a) G_\beta(z) \quad \text{with} \tag{5.8a}$$

$$G_\beta(z) = \sum_{0 \le h \in L} f_\beta(h) \mathbf{e}\big(\mathrm{tr}(hz)\big). \tag{5.8b}$$

Thus $F_0(-m;\, L,\, a,\, z)$ is a polynomial in a as stated in (iv). This argument is basically valid for F in place of F_0, but the functions corresponding to G_β in that case may depend on a. To avoid that difficulty, we first take a compact subset A of V and restrict a to A. As shown in the proof of Lemma 5.2, we can find a subset M of L independent of a such that

$$\big\{h \in L \,\big|\, h > 0,\, h + a > 0\big\} = M \sqcup K_a,$$

with a finite set K_a for each $a \in A$. Then, taking F in place of F_0, we obtain, for $a \in A$,

$$F(-m;\, L,\, a,\, z) = \sum_{\beta \in B} \beta(a) H_\beta(z) \quad \text{with} \tag{5.9a}$$

$$H_\beta(z) = \sum_{h \in K_a} f_\beta(h) \mathbf{e}\big(\mathrm{tr}(hz)\big) + \sum_{h \in M} f_\beta(h) \mathbf{e}\big(\mathrm{tr}(hz)\big). \tag{5.9b}$$

Thus the statement about $F(-m;\, L,\, a,\, z)$ in (iv) must be understood in the sense of (5.9a, b). It is a polynomial in a whose coefficients $H_\beta(z)$ is the sum of a "principal part" that is independent of a and a finite sum depending on a.

As for the value of Φ, from (5.7) we see that Φ is an entire functions of s. Also $\Gamma_n(s)^{-1}$ is nonzero for $(n-1)/2 < s \in \mathbf{R}$. Thus $\Phi(\kappa + m;\, L',\, a,\, z)$ is a nonzero constant times $F(-m;\, L,\, a,\, z)$, and so is a polynomial in a in the sense explained above.

5.4. Let us add some remarks. Clearly F_0 of (5.5) is a natural generalization of (0.1), but we introduced F and Φ as in (5.4) and (5.3), as we think they are natural objects of study closely related to (5.5). It must be remembered, however, that (5.5) includes (0.1) as a special case only if $|\gamma| < 1$. To define something like (5.5) that includes (0.1) with $|\gamma| = 1$ is one of the open problems in this area.

Next, there are four classical types of domains of positivity associated with tube domains discussed in [S82]. Our V, P, and $\mathfrak{H}$ in this section belong to the easiest type. We can in fact define the analogues of (5.3), (5.4), and (5.5) for all three other types of domains, and prove the results similar to Theorem 5.3 in those cases.

As to the nature of the polynomials in the variable a obtained in Theorem 5.3(iv), we do not have their description as explicit as what we know about $E_{c,m}(t)$. Still, we can show that they are of a rather special kind. For that purpose we need a matrix of differential operators $\partial_a = (\partial_{ij})_{i,j=1}^n$ on V as folows. Taking a variable symmetric matrix $a = (a_{ij})$ on V, we put $\partial_{ii} = \partial/\partial a_{ii}$ and $\partial_{ij} = 2^{-1}\partial/\partial a_{ij}$ for $i \neq j$. Then for every $\varphi \in S_d$ we can define a diffrential operator $\varphi(\partial_a)$. In particular, taking $\varphi(a) = \det(a)$, we put

$$\Delta_a = \det(\partial_a) = \sum_\sigma \operatorname{sgn}(\sigma)\partial_{1\sigma(1)} \cdots \partial_{n\sigma(n)}, \tag{5.10}$$

where σ runs over all permutations of $\{1, \ldots, n\}$. It is well known that

$$\Delta_a\bigl(\det(a)^s\bigr) = \prod_{k=0}^{n-1}(s + k/2) \cdot \det(a)^{s-1}. \tag{5.11}$$

This is a special case of a general formula on $\varphi(\partial_a)\det(z)^s$ for $\varphi \in S_d$ given in [S84].

Fixing L and z, for $0 \le m \in \mathbf{Z}$ put

$$\mathscr{E}_m(a) = F_0(-m;\, L,\, a,\, z). \tag{5.12}$$

We have shown that $\mathscr{E}_m$ is a polynomial of degree $\le mn$. Notice that $\mathscr{E}_0(a) = \sum_{0 \le h \in L} \mathbf{e}\bigl(\operatorname{tr}(hz)\bigr)$. From (5.8) and (5.11) we obtain

$$\Delta_a \mathscr{E}_m(a) = \prod_{k=0}^{n-1}(m + k/2) \cdot \mathscr{E}_{m-1}(a). \tag{5.13}$$

This is a generalization of the formula $(d/dt)E_{c,m}(t) = mE_{c,m-1}(t)$, noted in [S07, (4.3c)].

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Locally Well Generated Homotopy Categories of Complexes

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Abstract. We show that the homotopy category of complexes $\mathbf{K}(\mathcal{B})$ over any finitely accessible additive category $\mathcal{B}$ is locally well generated. That is, any localizing subcategory $\mathcal{L}$ in $\mathbf{K}(\mathcal{B})$ which is generated by a set is well generated in the sense of Neeman. We also show that $\mathbf{K}(\mathcal{B})$ itself being well generated is equivalent to $\mathcal{B}$ being pure semisimple, a concept which naturally generalizes right pure semisimplicity of a ring R for $\mathcal{B} = \text{Mod-}R$.

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Introduction

The main motivation for this paper is to study when the homotopy category of complexes $\mathbf{K}(\mathcal{B})$ over an additive category $\mathcal{B}$ is compactly generated or, more generally, well generated.

In the last few decades, the theory of compactly generated triangulated categories has become an important tool unifying concepts from various fields of mathematics. Standard examples are the unbounded derived category of a ring or the stable homotopy category of spectra. The key property of such a category $\mathcal{T}$ is the Brown Representability Theorem, cf. [30, 25], originally due to Brown [9]:

> Any contravariant cohomological functor $F : \mathcal{T} \to \text{Ab}$ which sends coproducts to products is representable.

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This theorem is an important tool and has been used in several places. We mention Neeman's proof of the Grothendieck Duality Theorem [30], Krause's work on the Telescope Conjecture [28, 24], or Keller's representation theorem for algebraic compactly generated triangulated categories [23].
Recently, there has been a growing interest in giving criteria for certain homotopy categories $\mathbf{K}(\mathcal{B})$ to be compactly generated, [15, 20, 29, 31]. Here, $\mathcal{B}$ typically was a suitable subcategory of a module category. The main reason for studying such homotopy categories were results concerning the Grothendieck Duality Theorem [17, 31] and relative homological algebra [19]. There is, however, a conceptual reason, too. Namely, every algebraic triangulated category is triangle equivalent to a full subcategory of some homotopy category, [25, §7.5].
It turned out when studying the homotopy category of complexes of projective modules over a ring R in [31] that it is useful to consider well generated triangulated categories in this context. More precisely, $\mathbf{K}(\text{Proj-}R)$ is always well generated, but may not be compactly generated. Well generated categories have been defined by Neeman [32] in a natural attempt to extend results such as the Brown Representability from compactly generated triangulated categories to a wider class of triangulated categories.

Although one has already known for some time that there exist rather natural triangulated categories, such as the homotopy category of complexes of abelian groups, which are not even well generated, one has typically viewed those as rare and exceptional cases.
We will give some arguments to show that this interpretation is not very accurate. First, the categories $\mathbf{K}(\text{Mod-}R)$ for a ring R are rarely well generated. It happens if and only if R is right pure semisimple, which establishes the converse of [15, §4 (3), p. 17]. Moreover, we generalize this result to the homotopy categories $\mathbf{K}(\mathcal{B})$ with $\mathcal{B}$ additive finitely accessible. This way, we obtain a fairly complete answer regarding when $\mathbf{K}(\text{Flat-}R)$ is compactly or well generated, see [15, Question 4.2].
We also give a partial remedy for the typical failure of $\mathbf{K}(\mathcal{B})$ to be well generated. Roughly speaking, the main problem with $\mathbf{K}(\mathcal{B})$, where $\mathcal{B}$ is finitely accessible, is that it may not have any set of generators at all. But if we take a localizing subcategory $\mathcal{L}$ generated by any set of objects, it will automatically be well generated. We will call a triangulated category with this property locally well generated.
We will also give basic properties of locally well generated categories and see that some of the usual results regarding localization hold in the new setting. For example, any localizing subcategory generated by a set of objects is realized as the kernel of a localization endofunctor. This version of a Bousfield localization theorem generalizes [26, §7.2] and [2, 5.7]. However, one has to be more careful. The Brown Representability theorem as stated above does not work for locally well generated categories in general, and there are localizing subcategories which are not associated to any localization endofunctor. We illustrate this in Example 3.7.

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1. Preliminaries

Let $\mathcal{T}$ be a triangulated category. A triangulated subcategory $\mathcal{S} \subseteq \mathcal{T}$ is called *thick* if, whenever $X \amalg Y \in \mathcal{S}$, then also $X \in \mathcal{S}$. From now on, we will assume that $\mathcal{T}$ has arbitrary (set-indexed) coproducts. A full triangulated subcategory $\mathcal{L} \subseteq \mathcal{T}$ is called *localizing* if it is closed under forming coproducts. Note that by [32, 1.6.8], $\mathcal{T}$ has splitting idempotents and any localizing subcategory $\mathcal{L} \subseteq \mathcal{T}$ is thick.

If $\mathcal{S}$ is any class of objects of $\mathcal{T}$, we denote by $\operatorname{Loc}\mathcal{S}$ the smallest localizing subcategory of $\mathcal{T}$ which contains $\mathcal{S}$. In other words, $\operatorname{Loc}\mathcal{S}$ is the closure of $\mathcal{S}$ under shifts, coproducts and triangle completions.

Given $\mathcal{T}$ and a localizing subcategory $\mathcal{L} \subseteq \mathcal{T}$, one can construct the so-called *Verdier quotient* $\mathcal{T}/\mathcal{L}$ by formally inverting in $\mathcal{T}$ all morphisms in the class $\Sigma(\mathcal{L})$ defined as

$$\Sigma(\mathcal{L}) = \{f \mid \exists \text{ triangle } X \xrightarrow{f} Y \to Z \to X[1] \text{ in } \mathcal{T} \text{ such that } Z \in \mathcal{L}\}.$$

It is a well known fact that the Verdier quotient always has coproducts, admits a natural triangulated structure, and the canonical localization functor $Q : \mathcal{T} \to \mathcal{T}/\mathcal{L}$ is exact and preserves coproducts, [32, Chapter 2]. However, one has to be careful, since $\mathcal{T}/\mathcal{L}$ might not be a usual category in the sense that the homomorphism spaces might be proper classes rather than sets. This fact, although often inessential and neglected, as $\mathcal{T}/\mathcal{L}$ has a very straightforward and constructive description, may nevertheless have important consequences in some cases; see eg. [6].

Let $L : \mathcal{T} \to \mathcal{T}$ be an exact endofunctor of $\mathcal{T}$. Then L is called a *localization functor* if there exists a natural transformation $\eta : \mathrm{Id}_{\mathcal{T}} \to L$ such that $L\eta_X = \eta_{LX}$ and $\eta_{LX} : LX \to L^2X$ is an isomorphism for each $X \in \mathcal{T}$.

It is easy to check that the full subcategory $\operatorname{Ker} L$ of $\mathcal{T}$ given by

$$\operatorname{Ker} L = \{X \in \mathcal{T} \mid LX = 0\}$$

is always localizing [2, 1.2]. Moreover, there is a canonical triangle equivalence between $\mathcal{T}/\operatorname{Ker} L$ and $\operatorname{Im} L$, the essential image of L; see [32, 9.1.16] or [26, 4.9.1]. This among other things implies that all morphism spaces in $\mathcal{T}/\operatorname{Ker} L$ are sets. Note that although $\operatorname{Im} L$ has coproducts as a category, it might *not* be closed under coproducts in $\mathcal{T}$. This type of localization, coming from a localization functor, is often referred to as *Bousfield localization.* However, not every localizing subcategory $\mathcal{L}$ is realized as the kernel of a localization functor, [6, 1.3]. Namely, $\mathcal{L}$ is of the form $\operatorname{Ker} L$ for some localization functor if and only if the inclusion $\mathcal{L} \to \mathcal{T}$ has a right adjoint, [2, 1.6].

A central concept in this paper is that of a well generated triangulated category. Let κ be a regular cardinal number. An object Y in a category with arbitrary coproducts is called κ–*small* provided that every morphism of the form

$$Y \longrightarrow \coprod_{i\in I} X_i$$

factorizes through a subcoproduct $\coprod_{i\in J} X_i$ with $|J| < \kappa$.

DEFINITION 1.1. Let $\mathcal{T}$ be a triangulated category with arbitrary coproducts and κ be a regular cardinal. Then $\mathcal{T}$ is called κ–*well generated* provided there is a set $\mathcal{S}$ of objects of $\mathcal{T}$ satisfying the following conditions:

(1) If $X \in \mathcal{T}$ such that $\mathcal{T}(Y, X) = 0$ for each $Y \in \mathcal{S}$, then $X = 0$;
(2) Each object $Y \in \mathcal{S}$ is κ–small;
(3) For any morphism in $\mathcal{T}$ of the form $f : Y \to \coprod_{i\in I} X_i$ with $Y \in \mathcal{S}$, there exists a family of morphisms $f_i : Y_i \to X_i$ such that $Y_i \in \mathcal{S}$ for each $i \in I$ and f factorizes as

$$Y \longrightarrow \coprod_{i\in I} Y_i \xrightarrow{\coprod f_i} \coprod_{i\in I} X_i.$$

The category $\mathcal{T}$ is called *well generated* if it is κ–well generated for some regular cardinal κ.

This definition differs to some extent from Neeman's original definition in [32, 8.1.7]. The equivalence between the two follows from [27, Theorem A] and [27, Lemmas 4 and 5]. Note that if $\kappa = \aleph_0$, then condition (3) is vacuous and $\aleph_0$–well generated triangulated categories are precisely the *compactly generated* triangulated categories in the usual sense.
The key property of well generated categories is that the Brown Representability Theorem holds:

PROPOSITION 1.2. [32, 8.3.3] *Let $\mathcal{T}$ be a well generated triangulated category. Then:*

(1) *Any contravariant cohomological functor $F : \mathcal{T} \to \mathrm{Ab}$ which takes coproducts to products is, up to isomorphism, of the form $\mathcal{T}(-, X)$ for some $X \in \mathcal{T}$.*
(2) *If $\mathcal{S}$ is a set of objects of $\mathcal{T}$ which meets assumptions* (1), (2) *and* (3) *of Definition 1.1 for some cardinal κ, then $\mathcal{T} = \mathrm{Loc}\,\mathcal{S}$.*

Next we turn our attention to categories of complexes. Let $\mathcal{B}$ be an additive category. Using a standard notation, we denote by $\mathbf{C}(\mathcal{B})$ the category of chain complexes

$$X : \qquad \cdots \to X^{n-1} \xrightarrow{d^{n-1}} X^n \xrightarrow{d^n} X^{n+1} \to \dots,$$

of objects of $\mathcal{B}$. By $\mathbf{K}(\mathcal{B})$, we denote the factor-category of $\mathbf{C}(\mathcal{B})$ modulo the ideal of null-homotopic chain complex morphisms. It is well known that $\mathbf{K}(\mathcal{B})$ has a triangulated structure where triangle completions are constructed using mapping cones (see for example [14, Chapter I]). Moreover, if $\mathcal{B}$ has arbitrary coproducts, so have them both $\mathbf{C}(\mathcal{B})$ and $\mathbf{K}(\mathcal{B})$, and the canonical functor $\mathbf{C}(\mathcal{B}) \to \mathbf{K}(\mathcal{B})$ preserves coproducts.

We will often take for $\mathcal{B}$ module categories or their subcategories. In this case, R will denote an associative unital ring and Mod-R the category of all (unital) right R–modules. By Proj-R and Flat-R we denote, respectively, the full subcategories of projective and flat R–modules.

In fact, our considerations will usually work in a more general setting. Let $\mathcal{A}$ be a skeletally small additive category and Mod-$\mathcal{A}$ be the category of all contravariant additive functors $\mathcal{A} \to \mathrm{Ab}$. We will call such functors *right $\mathcal{A}$–modules*. Then Mod-$\mathcal{A}$ shares many formal properties with usual module categories. We refer to [18, Appendix B] for more details. Correspondingly, we denote by Proj-$\mathcal{A}$ the full subcategory of projective functors and by Flat-$\mathcal{A}$ the category of flat functors. We discuss the categories of the form Flat-$\mathcal{A}$ more in detail in Section 4 since those are, up to equivalence, precisely the so called additive finitely accessible categories. Many natural abelian categories are of this form.

Finally, we spend a few words on set-theoretic considerations. All our proofs work in ZFC with an extra technical assumption: the axiom of choice for proper classes. The latter assumption has no algebraic significance, it is only used to keep arguments simple in the following case:

Let $F : \mathcal{C} \to \mathcal{D}$ be a covariant additive functor. If we know, for example by the Brown Representability Theorem, that the composition of functors

$$\mathcal{C} \xrightarrow{\ F\ } \mathcal{D} \xrightarrow{\mathcal{D}(-,X)} \mathrm{Ab}$$

is representable for each $X \in \mathcal{D}$, we would like to conclude that F has a right adjoint $G : \mathcal{D} \to \mathcal{C}$. In order to do that, we must for each $Y \in \mathcal{C}$ *choose* one particular value for GY from a class of mutually isomorphic candidates.

2. Pure semisiplicity

A relatively straightforward but crucial obstacle causing a homotopy category of complexes $\mathbf{K}(\mathcal{B})$ not to be well generated is that the additive base category $\mathcal{B}$ is not pure semisimple. Here, we use the following very general definition:

Definition 2.1. An additive category $\mathcal{B}$ with arbitrary coproducts is called *pure semisimple* if it has an additive generator. That is, there is an object $X \in \mathcal{B}$ such that $\mathcal{B} = \mathrm{Add}X$, where $\mathrm{Add}X$ stands for the full subcategory formed by all objects which are summands in (possibly infinite) coproducts of copies of X.

The term is inspired by the case $\mathcal{B} = $ Mod-R, where we have the following proposition:

Proposition 2.2. *A ring R is right pure semisimple (that is, each pure monomorphism between right R–modules splits) if and only if* Mod-R *is pure semisimple in the sense of Definition 2.1.*

Proof. If every pure monomorphism in Mod-R splits, then also every pure epimorphism splits. That is, every module is pure projective, or equivalently a summand in a direct sum of finitely presented modules. By a theorem of

Kaplansky, [21, Theorem 1], it follows that every module is a direct sum of countably generated modules. Hence, Mod-R is pure semisimple according to our definition. In fact, one can show more in this case: Every module is even a direct sum of finitely presented modules; see for example [16] or [18, App. B]. Let us conversely assume that Mod-R is a pure semisimple additive category. Using [3, Theorem 26.1], which is a variation of [21, Theorem 1] for higher cardinalities, we see that if Mod-$R = \mathrm{Add}X$ for some κ–generated module X, then each module in Mod-R is a direct sum of λ–generated modules where $\lambda = \max(\kappa, \aleph_0)$. This fact implies that every module is Σ–pure injective, [12]. In particular, each pure monomorphism in Mod-R splits and R is right pure semisimple. □

If R is an artin algebra, then the conditions of Proposition 2.2 are well-known to be further equivalent to R being of finite representation type; see [4, Theorem A]. For more details and references on this topic, we also refer to [16]. It turns out that the pure semisimplicity condition has a nice interpretation for finitely accessible additive categories as well. We will discuss this more in detail in Section 4.

For giving a connection between pure semisimplicity of $\mathcal{B}$ and properties of $\mathbf{K}(\mathcal{B})$, we recall a structure result for the so-called contractible complexes in $\mathbf{C}(\mathcal{B})$. A complex $Y \in \mathbf{C}(\mathcal{B})$ is *contractible* if it is mapped to a zero object under $\mathbf{C}(\mathcal{B}) \to \mathbf{K}(\mathcal{B})$. It is clear that the complexes of the form

$$I_{X,n}: \qquad \cdots \to 0 \to 0 \to X = X \to 0 \to 0 \to \dots,$$

such that the first X is in degree n, are contractible. Moreover, all other contractible complexes are obtained in the following way:

LEMMA 2.3. *Let $\mathcal{B}$ be an additive category with splitting idempotents and $Y \in \mathbf{C}(\mathcal{B})$. Then the following are equivalent:*

(1) *Y is contractible;*
(2) *Y is isomorphic in $\mathbf{C}(\mathcal{B})$ to a complex of the form $\coprod_{n\in\mathbb{Z}} I_{X_n,n}$.*

Proof. (2) $\implies$ (1). This is trivial given the fact that the functor $\mathbf{C}(\mathcal{B}) \to \mathbf{K}(\mathcal{B})$ preserves those componentwise coproducts of complexes which exist in $\mathbf{C}(\mathcal{B})$.
(1) $\implies$ (2). Let us fix a contractible complex in $\mathbf{K}(\mathcal{B})$:

$$Y: \qquad \dots \xrightarrow{d^{n-2}} Y^{n-1} \xrightarrow{d^{n-1}} Y^n \xrightarrow{d^n} Y^{n+1} \xrightarrow{d^{n+1}} \dots.$$

By definition, the identity morphism of Y is homotopy equivalent to the zero morphism in $\mathbf{C}(\mathcal{B})$, so there are morphisms $s^n : Y^n \to Y^{n-1}$ in $\mathcal{B}$ such that

$$1_{Y^n} = d^{n-1}s^n + s^{n+1}d^n.$$

When composing with d^n, we get $d^n = d^n s^{n+1} d^n$, so $s^{n+1}d^n : Y^n \to Y^n$ is idempotent in $\mathcal{B}$ for each $n \in \mathbb{Z}$. Hence there are morphisms $p^n : Y^n \to X_n$ and $j^n : X_n \to Y^n$ in $\mathcal{B}$ such that $p^n j^n = 1_{X_n}$ and $j^n p^n = s^{n+1}d^n$. Let us denote by $f^n : X_{n-1} \amalg X_n \to Y^n$ and $g^n : Y^n \to X_{n-1} \amalg X_n$ the morphisms defined as follows:

$$f^n = (d^{n-1}j^{n-1}, j^n), \quad \text{and} \quad g^n = \begin{pmatrix} p^{n-1}s^n \\ p^n \end{pmatrix}.$$

Using the identities above, it is easy to check that $f^n g^n = 1_{Y^n}$ and $g^n f^n$ is an isomorphism in $\mathcal{B}$ for each n. Therefore, both f^n and g^n are isomorphisms and $g^n f^n$ is the identity morphism. Finally, it is straightforward to check that the family of morphisms $(f_n \mid n \in \mathbb{Z})$ induces an (iso)morphism $f : \coprod_{n \in Z} I_{X_n,n} \to Y$ in $\mathbf{C}(\mathcal{B})$. □

It is not difficult to see that the condition of $\mathcal{B}$ having splitting idempotents is really necessary in Lemma 2.3. However, there is a standard construction which allows us to amend $\mathcal{B}$ with the missing summands if $\mathcal{B}$ does not have splitting idempotents.

Definition 2.4. Let $\mathcal{B}$ be an additive category. Then an additive category $\bar{\mathcal{B}}$ is called an *idempotent completion* of $\mathcal{B}$ if

(1) $\bar{\mathcal{B}}$ has splitting idempotents;
(2) $\mathcal{B}$ is a full subcategory of $\bar{\mathcal{B}}$;
(3) Every object in $\bar{\mathcal{B}}$ is a direct summand of an object in $\mathcal{B}$.

It is a classical result that idempotent completions always exist. We refer for example to [5, §1] for a particular construction. Moreover, it is well-known that if $\mathcal{B}$ has arbitrary coproducts, then also $\bar{\mathcal{B}}$ has them and they are compatible with coproducts in $\mathcal{B}$.
Now we can state the main result of the section showing that for $\mathbf{K}(\mathcal{B})$ being generated by a set (and, in particular, for $\mathbf{K}(\mathcal{B})$ being well generated), the category $\mathcal{B}$ is necessarily pure semisimple.

Theorem 2.5. *Let $\mathcal{B}$ be an additive category with arbitrary coproducts and assume that there is a set of objects $\mathcal{S} \subseteq \mathbf{K}(\mathcal{B})$ such that $\mathbf{K}(\mathcal{B}) = \operatorname{Loc}\mathcal{S}$. Then $\mathcal{B}$ is pure semisimple.*

Proof. Note that we can replace $\mathcal{S}$ by a singleton $\{Y\}$; take for instance $Y = \coprod_{Z \in \mathcal{S}} Z$. Let us denote by $X \in \mathcal{B}$ the coproduct $\coprod_{n \in \mathbb{Z}} Y^n$ of all components of Y. We will show that $\mathcal{B} = \operatorname{Add}X$. First, we claim that $\mathbf{K}(\operatorname{Add}X)$ is a dense subcategory of $\mathbf{K}(\mathcal{B})$, that is, each object in $\mathbf{K}(\mathcal{B})$ is isomorphic to one in $\mathbf{K}(\operatorname{Add}X)$. Indeed, $Y \in \mathbf{K}(\operatorname{Add}X)$ and one easily checks that the closure of $\mathbf{K}(\operatorname{Add}X)$ under taking isomorphic objects in $\mathbf{K}(\mathcal{B})$ is a localizing subcategory. Hence $\mathbf{K}(\operatorname{Add}X)$ is dense in $\mathbf{K}(\mathcal{B})$ and the claim is proved.
Suppose for the moment that $\mathcal{B}$ has splitting idempotents. If we identify $\mathcal{B}$ with the full subcategory of $\mathbf{K}(\mathcal{B})$ formed by complexes concentrated in degree zero, we have proved that each object $Z \in \mathcal{B}$ is isomorphic to a complex $Q \in \mathbf{K}(\operatorname{Add}X)$. That is, there is a chain complex homomorphism $f : Z \to Q$ such that $Q \in \mathbf{C}(\operatorname{Add}X)$ and f becomes an isomorphism in $\mathbf{K}(\mathcal{B})$. In particular,

the mapping cone C_f of f is contractible:

$$C_f: \qquad \dots \longrightarrow Q^{-3} \xrightarrow{d^{-3}} Q^{-2} \xrightarrow{\binom{d^{-2}}{0}} Q^{-1} \amalg Z \xrightarrow{(d^{-1}, f^0)} Q^0 \xrightarrow{d^0} Q^1 \longrightarrow \dots$$

Here, f^0 is the degree 0 component of f. Consequently, Lemma 2.3 yields the following commutative diagram in $\mathcal{B}$ with isomorphisms in columns:

$$\begin{array}{ccccc} Q^{-2} & \xrightarrow{\binom{d^{-2}}{0}} & Q^{-1} \amalg Z & \xrightarrow{(d^{-1}, f^0)} & Q^0 \\ \cong\downarrow & & \cong\downarrow & & \cong\downarrow \\ U \amalg V & \xrightarrow{\left(\begin{smallmatrix}0 & 1\\ 0 & 0\end{smallmatrix}\right)} & V \amalg W & \xrightarrow{\left(\begin{smallmatrix}0 & 1\\ 0 & 0\end{smallmatrix}\right)} & W \amalg Z \end{array}$$

It follows that V, W and also $Q^{-1} \amalg Z$ and Z are in $\operatorname{Add} X$. Hence $\mathcal{B} = \operatorname{Add} X$. Finally, let $\mathcal{B}$ be a general additive category with coproducts and $\bar{\mathcal{B}}$ be its idempotent completion. From the fact that $\mathbf{K}(\mathcal{B})$ has splitting idempotents, [32, 1.6.8], one easily sees that the full embedding $\mathbf{K}(\mathcal{B}) \to \mathbf{K}(\bar{\mathcal{B}})$ is dense. We already know that if $\mathbf{K}(\mathcal{B}) = \operatorname{Loc} \mathcal{S}$ for a set $\mathcal{S}$, then $\bar{\mathcal{B}} = \operatorname{Add} X$ for some $X \in \bar{\mathcal{B}}$. In fact, we can take $X \in \mathcal{B}$ by the above construction. But then clearly $\mathcal{B} = \operatorname{Add} X$ when the additive closure is taken in $\mathcal{B}$. Hence $\mathcal{B}$ is pure semisimple. □

Remark. When studying well generated triangulated categories, an important role is played by so-called κ–localizing subcategories, see [32, 26]. We recall that given a cardinal number κ, a *κ–coproduct* is a coproduct with fewer than κ summands. If $\mathcal{T}$ is a triangulated category with arbitrary κ–coproducts, a thick subcategory $\mathcal{L} \subseteq \mathcal{T}$ is called *κ–localizing* if it is closed under taking κ–coproducts. In this context, one can state the following "bounded" version of Theorem 2.5:
Let κ be an uncountable regular cardinal and $\mathcal{B}$ be an additive category with κ–coproducts. If $\mathbf{K}(\mathcal{B})$ is generated as a κ–localizing subcategory by a set $\mathcal{S}$ of fewer than κ objects, then there is $X \in \mathcal{B}$ such that every object of $\mathcal{B}$ is a summand in a κ–coproduct of copies of X.

Note that Theorem 2.5 gives immediately a wide range of examples of categories which are not well generated. For instance, $\mathbf{K}(\text{Mod-}R)$ is not well generated for any ring R which is not right pure semisimple. One can take $R = \mathbb{Z}$ or $R = k(\cdot \rightrightarrows \cdot)$, the Kronecker algebra over a field k. The fact that $\mathbf{K}(\text{Ab})$ is not well generated was first observed by Neeman, [32, E.3.2], using different arguments. In fact, we can state the following proposition, which we later generalize in Section 5:

Proposition 2.6. *Let R be a ring. Then the following are equivalent:*

(1) $\mathbf{K}(\text{Mod-}R)$ *is well generated;*
(2) $\mathbf{K}(\text{Mod-}R)$ *is compactly generated;*
(3) R *is right pure semisimple.*

If R is an artin algebra, the conditions are further equivalent to:

(4) R *is of finite representation type.*

Proof. (2) $\implies$ (1) is clear, as compactly generated is the same as $\aleph_0$–well generated. (1) $\implies$ (3) follows by Theorem 2.5 and Proposition 2.2. (3) $\implies$ (2) has been proved by Holm and Jørgensen, [15, §4 (3), p. 17]. Finally, the equivalence between (3) and (4) is due to Auslander, [4, Theorem A]. □

3. Locally well generated triangulated categories

We have seen in the last section that a triangulated category of the form $\mathbf{K}(\text{Mod-}R)$ is often not well generated. One might get an impression that handling such categories is hopeless, but the main problem here actually is that the category is very big in the sense that it is not generated by any set. Otherwise, it has a very reasonable structure. We shall see that it is locally well generated in the following sense:

Definition 3.1. A triangulated category $\mathcal{T}$ with arbitrary coproducts is called *locally well generated* if $\operatorname{Loc}\mathcal{S}$ is well generated for any set $\mathcal{S}$ of objects of $\mathcal{T}$.

In fact, we prove that $\mathbf{K}(\text{Mod-}\mathcal{A})$ is locally well generated for any skeletally small additive category $\mathcal{A}$. To this end, we first need to be able to measure the size of modules and complexes.

Definition 3.2. Let $\mathcal{A}$ be a skeletally small additive category and $M \in \text{Mod-}\mathcal{A}$. Recall that M is a contravariant additive functor $\mathcal{A} \to \text{Ab}$ by definition. Then the *cardinality of* M, denoted by $|M|$, is defined as

$$|M| = \sum_{A \in \mathcal{S}} |M(A)|,$$

where $|M(A)|$ is just the usual cardinality of the group $M(A)$ and $\mathcal{S}$ is a fixed representative set for isomorphism classes of objects from $\mathcal{A}$. The *cardinality of a complex* $Y = (Y^n, d^n) \in \mathbf{K}(\text{Mod-}\mathcal{A})$ is defined as

$$|Y| = \sum_{n \in \mathbb{Z}} |Y^n|.$$

It is not so difficult to see that the category of all complexes whose cardinalities are bounded by a given regular cardinal always gives rise to a well-generated subcategory of $\mathbf{K}(\text{Mod-}\mathcal{A})$:

Lemma 3.3. *Let $\mathcal{A}$ be a skeletally small additive category and κ be an infinite cardinal. Then the full subcategory $\mathcal{S}_\kappa$ formed by all complexes of cardinality less than κ meets conditions* (2) *and* (3) *of Definition 1.1.*
In particular, $\mathcal{T}_\kappa = \operatorname{Loc}\mathcal{S}_\kappa$ is a κ–well generated subcategory of $\mathbf{K}(\text{Mod-}\mathcal{A})$ for any regular cardinal κ.

Proof. Let $Y \in \mathbf{K}(\text{Mod-}\mathcal{A})$ such that $|Y| < \kappa$. If $(Z_i \mid i \in I)$ is an arbitrary family of complexes in $\mathbf{K}(\text{Mod-}\mathcal{A})$, we can construct their coproduct as a componentwise coproduct in $\mathbf{C}(\text{Mod-}\mathcal{A})$. Then whenever $f : Y \to \coprod_{i \in I} Z_i$ is a morphism in $\mathbf{C}(\text{Mod-}\mathcal{A})$, it is straightforward to see that f factorizes through $\coprod_{i \in J} Z_i$ for some $J \subseteq I$ of cardinality less than κ. Hence Y is κ–small in $\mathbf{K}(\text{Mod-}\mathcal{A})$.

Regarding part (3) of Definition 1.1, consider a morphism $f : Y \to \coprod_{i\in I} Z_i$. We have the following factorization in the abelian category of complexes $\mathbf{C}(\text{Mod-}\mathcal{A})$:

$$Y \xrightarrow{(f_i)} \coprod_{i\in I} \operatorname{Im} f_i \xrightarrow{j} \coprod_{i\in I} Z_i.$$

Here, $f_i : Y \to Z_i$ are the compositions of f with the canonical projections $\pi_i : \coprod_{i'\in I} Z_{i'} \to Z_i$, and j stands for the obvious inclusion. It is easy to see that $|\operatorname{Im} f_i| < \kappa$ for each $i \in I$ and that the morphism j is a coproduct of the inclusions $\operatorname{Im} f_i \to Z_i$. Hence (3) is satisfied.
For the second part, let κ be regular and $\mathcal{T}_\kappa = \operatorname{Loc} \mathcal{S}_\kappa$. Let us denote by $\mathcal{S}'$ a representative set of objects in $\mathcal{S}_\kappa$. It only remains to prove that $\mathcal{S}'$ satisfies condition (1) of Definition 1.1, which is rather easy. Namely, let $X \in \mathcal{T}_\kappa$ such that $\mathcal{T}_\kappa(Y, X) = 0$ for each $Y \in \mathcal{S}'$. Then $\mathcal{T}' = \{Y \in \mathcal{T}_\kappa \mid \mathcal{T}_\kappa(Y, X) = 0\}$ defines a localizing subcategory of $\mathcal{T}_\kappa$ containing $\mathcal{S}_\kappa$. Hence, $\mathcal{T}' = \mathcal{T}_\kappa$ and $X = 0$. □

We will also need (a simplified version of) an important result, which is essentially contained already in [32]. It says that the property of being well generated is preserved when passing to any localizing subcategory generated by a set. In particular, every well generated category is locally well generated.

Proposition 3.4. [26, Theorem 7.2.1] *Let $\mathcal{T}$ be a well generated triangulated category and $\mathcal{S} \subseteq \mathcal{T}$ be a set of objects. Then* $\operatorname{Loc} \mathcal{S}$ *is a well generated triangulated category, too.*

Now, we are in a position to state a theorem which gives us a major source of examples of locally well generated triangulated categories.

Theorem 3.5. *Let $\mathcal{A}$ be a skeletally small additive category. Then the triangulated category* $\mathbf{K}(\text{Mod-}\mathcal{A})$ *is locally well generated.*

Proof. As in Lemma 3.3, we denote by $\mathcal{S}_\kappa$ the full subcategory of $\mathbf{K}(\text{Mod-}\mathcal{A})$ formed by complexes of cardinality less than κ and put $\mathcal{T}_\kappa = \operatorname{Loc} \mathcal{S}_\kappa$, the localizing class generated by $\mathcal{S}_\kappa$ in $\mathbf{K}(\text{Mod-}\mathcal{A})$. Then $\mathcal{T}_\kappa$ is (κ–)well generated for each regular cardinal κ by Lemma 3.3 and clearly

$$\mathbf{K}(\text{Mod-}\mathcal{A}) = \bigcup_{\kappa \text{ regular}} \mathcal{S}_\kappa = \bigcup_{\kappa \text{ regular}} \mathcal{T}_\kappa.$$

Now, if $\mathcal{S} \subseteq \mathbf{K}(\text{Mod-}\mathcal{A})$ is a set of objects, then $\mathcal{S} \subseteq \mathcal{T}_\kappa$ for some κ. Hence also $\operatorname{Loc} \mathcal{S} \subseteq \mathcal{T}_\kappa$ and $\operatorname{Loc} \mathcal{S}$ is well generated by Proposition 3.4. It follows that $\mathbf{K}(\text{Mod-}\mathcal{A})$ is locally well generated. □

Having obtained a large class of examples of locally well generated triangulated categories, one might ask for some basic properties of such categories. We will prove a version of the so-called Bousfield Localization Theorem here:

Proposition 3.6. *Let $\mathcal{T}$ be a locally well generated triangulated category and $\mathcal{S} \subseteq \mathcal{T}$ be a set of objects. Then $\mathcal{T}/\operatorname{Loc} \mathcal{S}$ is a Bousfield localization; that* *is, there is a localization functor* $L : \mathcal{T} \to \mathcal{T}$ *such that* $\operatorname{Ker} L = \operatorname{Loc} \mathcal{S}$*. In particular, we have*

$$\operatorname{Im} L = \{X \in \mathcal{T} \mid \mathcal{T}(Y, X) = 0 \text{ for each } Y \in \mathcal{S}\},$$

there is a canonical triangle equivalence between $\mathcal{T}/\operatorname{Loc}\mathcal{S}$ *and* $\operatorname{Im} L$ *given by the composition*

$$\operatorname{Im} L \xrightarrow{\subseteq} \mathcal{T} \xrightarrow{Q} \mathcal{T}/\operatorname{Loc}\mathcal{S},$$

and all morphism spaces in $\mathcal{T}/\operatorname{Loc}\mathcal{S}$ *are sets.*

Proof. The proof is rather standard. $\operatorname{Loc}\mathcal{S}$ is well generated, so it satisfies the Brown Representability Theorem (see Proposition 1.2). Hence the inclusion $\mathbf{i} : \operatorname{Loc}\mathcal{S} \to \mathcal{T}$ has a right adjoint by [32, 8.4.4]. The composition of this right adjoint with $\mathbf{i}$ gives a so-called colocalization functor $\Gamma : \mathcal{T} \to \mathcal{T}$ whose essential image is equal to $\operatorname{Loc}\mathcal{S}$. The definition of a colocalization functor is formally dual to the one of a localization functor; see [26, §4.12] for details. A well-known construction then yields a localization functor $L : \mathcal{T} \to \mathcal{T}$ such that $\operatorname{Ker} L = \operatorname{Loc}\mathcal{S}$. We refer to [32, 9.1.14] or [26, 4.12.1] for details. The rest follows from [32, 9.1.16] or [26, 4.9.1]. □

Remark. Proposition 3.6 has been proved before for well generated triangulated categories. This is implicitly contained for example in [26, §7.2]. It also generalizes more classical results, such as a corresponding statement for the derived category $\mathbf{D}(\mathcal{B})$ of a Grothendieck category $\mathcal{B}$, [2, 5.7]. To see this, one only needs to observe that $\mathbf{D}(\mathcal{B})$ is well generated, see [26, Example 7.7].

An obvious question is whether the Brown Representability Theorem also holds for locally well generated categories, as this was the crucial feature of well generated categories. Unfortunately, this is not the case in general, as the following example suggested by Henning Krause shows.

Example 3.7. According to [10, Exercise 1, p. 131], one can construct an abelian category $\mathcal{B}$ with some Ext-spaces being proper classes. Namely, let U be the class of all cardinals, and let $\mathcal{B} = \text{Mod-}\mathbb{Z}\langle U\rangle$, the category of all "modules over the free ring on the proper class of generators U." That is, an object X of $\mathcal{B}$ is an abelian group such that each $\kappa \in U$ has a $\mathbb{Z}$-linear action on X and this action is trivial for all but a set of cardinals. Such a category admits a valid set-theoretical description in ZFC. If we denote by $\mathbb{Z}$ the object of $\mathcal{B}$ whose underlying group is free of rank 1 and $\kappa \cdot \mathbb{Z} = 0$ for each $\kappa \in U$, then $\operatorname{Ext}^1_{\mathcal{B}}(\mathbb{Z}, \mathbb{Z})$ is a proper class (see also [26, 4.15] or [6, 1.1]).
Given the above description of objects of $\mathcal{B}$, one can easily adjust the proof of Theorem 3.5 to see that $\mathbf{K}(\mathcal{B})$ is locally well generated. Let $\mathbf{K}_{\mathrm{ac}}(\mathcal{B})$ stand for the full subcategory of all acyclic complexes in $\mathbf{K}(\mathcal{B})$. Then $\mathbf{K}_{\mathrm{ac}}(\mathcal{B})$ is clearly a localizing subcategory of $\mathbf{K}(\mathcal{B})$, hence locally well-generated.
It has been shown in [6] that $\mathbf{K}_{\mathrm{ac}}(\mathcal{B})$ does not satisfy the Brown Representability Theorem. In fact, one proved even more: $\mathbf{K}_{\mathrm{ac}}(\mathcal{B})$ is localizing in $\mathbf{K}(\mathcal{B})$, but it is not a kernel of any localization functor $L : \mathbf{K}(\mathcal{B}) \to \mathbf{K}(\mathcal{B})$. More

specifically, the composition of functors, the second of which is contravariant,

$$\mathbf{K}_{\mathrm{ac}}(\mathcal{B}) \xrightarrow{\subseteq} \mathbf{K}(\mathcal{B}) \xrightarrow{\mathbf{K}(\mathcal{B})(-,\mathbb{Z})} \mathrm{Ab}$$

is not representable by any object of $\mathbf{K}_{\mathrm{ac}}(\mathcal{B})$.

Yet another natural question is what other triangulated categories are locally well generated. A deeper analysis of this problem is left for future research, but we will see in Section 4 that $\mathbf{K}(\mathcal{B})$ is locally well generated for any finitely accessible additive category $\mathcal{B}$. For now, we will prove that the class of locally well generated triangulated categories is closed under some natural constructions. Let us start with a general lemma, which holds even if morphism spaces in the quotient $\mathcal{T}/\mathcal{L}$ are proper classes:

LEMMA 3.8. *Let $\mathcal{T}$ be a triangulated category and $\mathcal{L} \subseteq \mathcal{L}'$ be two localizing subcategories of $\mathcal{T}$. Then $\mathcal{L}'/\mathcal{L}$ is a localizing subcategory of $\mathcal{T}/\mathcal{L}$.*

Proof. It is easy to see that $\mathcal{L}'/\mathcal{L}$ is a full subcategory of $\mathcal{T}/\mathcal{L}$ which is closed under taking isomorphic objects, see [33, Théorème 4-2] or [22, Proposition 1.6.5]. The rest follows directly from the construction of $\mathcal{T}/\mathcal{L}$. □

Now we can show that taking localizing subcategories and localizing with respect to a set of objects preserves the locally well generated property.

PROPOSITION 3.9. *Let $\mathcal{T}$ be a locally well generated triangulated category.*

(1) *Any localizing subcategory $\mathcal{L}$ of $\mathcal{T}$ is itself locally well generated.*
(2) *The Verdier quotient $\mathcal{T}/\mathrm{Loc}\,\mathcal{S}$ is locally well generated for any set $\mathcal{S}$ of objects in $\mathcal{T}$.*

Proof. (1) is trivial. For (2), put $\mathcal{L} = \mathrm{Loc}\,\mathcal{S}$ and consider a set $\mathcal{C}$ of objects in $\mathcal{T}/\mathcal{L}$. We have to prove that the localizing subcategory generated by $\mathcal{C}$ in $\mathcal{T}/\mathcal{L}$ is well generated. Since the objects of $\mathcal{T}$ and $\mathcal{T}/\mathcal{L}$ coincide by definition, we can consider a localizing subcategory $\mathcal{L}' \subseteq \mathcal{T}$ defined by $\mathcal{L}' = \mathrm{Loc}\,(\mathcal{S} \cup \mathcal{C})$. One easily sees using Lemma 3.8 that $\mathcal{L}'/\mathcal{L} = \mathrm{Loc}\,\mathcal{C}$ in $\mathcal{T}/\mathcal{L}$. Since both $\mathcal{L}$ and $\mathcal{L}'$ are well generated by definition, so is $\mathcal{L}'/\mathcal{L}$ by [26, 7.2.1]. Hence $\mathcal{T}/\mathcal{L}$ is locally well generated. □

We conclude this section with an immediate consequence of Theorem 3.5 and Proposition 3.9, which will be useful in the next section:

COROLLARY 3.10. *Let $\mathcal{A}$ be a small additive category and $\mathcal{B}$ be a full subcategory of* Mod-$\mathcal{A}$ *which is closed under arbitrary coproducts. Then $\mathbf{K}(\mathcal{B})$ is locally well generated.*

4. FINITELY ACCESSIBLE ADDITIVE CATEGORIES

There is a natural generalization of module categories, namely the additive version of finitely accessible categories in the terminology of [1]. As we have seen, there is quite a lot of freedom to choose $\mathcal{B}$ in the above Corollary 3.10. We will use this fact and a standard trick to (seemingly) generalize Theorem 3.5

from module categories to finitely accessible additive categories. We start with a definition.

Definition 4.1. Let $\mathcal{B}$ be an additive category which admits arbitrary filtered colimits. Then:

- An object $X \in \mathcal{B}$ is called *finitely presentable* if the representable functor $\mathcal{B}(X, -) : \mathcal{B} \to \mathrm{Ab}$ preserves filtered colimits.
- The category $\mathcal{B}$ is called *finitely accessible* if there is a set $\mathcal{A}$ of finitely presentable objects from $\mathcal{B}$ such that every object in $\mathcal{B}$ is a filtered colimit of objects from $\mathcal{A}$.

Note that if $\mathcal{B}$ is finitely accessible, the full subcategory $\mathrm{fp}(\mathcal{B})$ of $\mathcal{B}$ formed by all finitely presentable objects in $\mathcal{B}$ is skeletally small, [1, 2.2]. Several other general properties of finitely accessible categories will follow from Proposition 4.2.

Finitely accessible categories occur at many occasions. The simplest and most natural example is the module category Mod-R over an associative unital ring. It is well-known that finitely presentable objects in Mod-R coincide with finitely presented R–modules in the usual sense. The same holds for Mod-$\mathcal{A}$, the category of modules over a small additive category $\mathcal{A}$. Motivated by representation theory, finitely accessible categories were studied by Crawley-Boevey [8] under the name locally finitely presented categories; see [8, §5] for further examples. The term from [8], however, may cause some confusion in the light of other definitions. Namely, Gabriel and Ulmer [11] have defined the concept of a *locally finitely presentable* category which is, in our terminology, a cocomplete finitely accessible category. As the latter concept has been used quite substantially in one of our main references, [26], we stick to the terminology of [1].

The crucial fact about finitely accessible additive categories is the following representation theorem:

Proposition 4.2. *The assignments*

$$\mathcal{A} \mapsto \mathrm{Flat}\text{-}\mathcal{A} \quad \textit{and} \quad \mathcal{B} \mapsto \mathrm{fp}(\mathcal{B})$$

form a bijective correspondence between

(1) *equivalence classes of skeletally small additive categories $\mathcal{A}$ with splitting idempotents, and*
(2) *equivalence classes of additive finitely accessible categories $\mathcal{B}$.*

Proof. See [8, §1.4]. □

Remark. The correspondence from Proposition 4.2 restricts, using [8, §2.2], to a bijection between equivalence classes of skeletally small additive categories with finite colimits (equivalently, with cokernels) and equivalence classes of locally finitely presentable categories in the sense of Gabriel and Ulmer [11].

One of the main results of this paper has now become a mere corollary of preceding results:

Theorem 4.3. *Let $\mathcal{B}$ be a finitely accessible additive category. Then $\mathbf{K}(\mathcal{B})$ is locally well generated.*

Proof. Let us put $\mathcal{A} = \mathrm{fp}(\mathcal{B})$, the full subcategory of $\mathcal{B}$ formed by all finitely presentable objects. Using Proposition 4.2, we see that $\mathcal{B}$ is equivalent to the category Flat-$\mathcal{A}$. The category $\mathbf{K}(\text{Flat-}\mathcal{A})$ is locally well generated by Corollary 3.10, and so must be $\mathbf{K}(\mathcal{B})$. □

The remaining question when $\mathbf{K}(\mathcal{B})$ is κ–well generated and which cardinals κ can occur will be answered in the next section. For now, we know by Theorem 2.5 that a necessary condition is that $\mathcal{B}$ be pure semisimple. In fact, we will show that this is also sufficient, but at the moment we will only give a better description of pure semisimple finitely accessible additive categories.

Proposition 4.4. *Let $\mathcal{B}$ be a finitely accessible additive category. Then the following are equivalent:*

(1) *$\mathcal{B}$ is pure semisimple in the sense of Definition 2.1;*
(2) *Each object in $\mathcal{B}$ is a coproduct of (indecomposable) finitely presentable objects;*
(3) *Each flat right $\mathcal{A}$–module is projective, where $\mathcal{A} = \mathrm{fp}(\mathcal{B})$.*

Proof. For the whole argument, we put $\mathcal{A} = \mathrm{fp}(\mathcal{B})$ and without loss of generality assume that $\mathcal{B} = \text{Flat-}\mathcal{A}$.
(1) $\implies$ (3). Assume that Flat-$\mathcal{A}$ is pure semisimple. As in the proof for Proposition 2.2, we can use a generalization [3, Theorem 26.1] of Kaplansky's theorem, to deduce that there is a cardinal number λ such that each flat $\mathcal{A}$–module is a direct sum of at most λ–generated flat $\mathcal{A}$–modules. The key step is then contained in [13, Corollary 3.6] which says that under the latter condition $\mathcal{A}$ is a right perfect category. That is, it satisfies the equivalent conditions of Bass' theorem [18, B.12] (or more precisely, its version for contravariant functors $\mathcal{A} \to \mathrm{Ab}$). One of the equivalent conditions is condition (3).
(3) $\implies$ (2). This is a consequence of Bass' theorem; see [18, B.13].
(2) $\implies$ (1). Trivial, $\mathcal{B} = \mathrm{Add}X$ where $X = \bigoplus_{Y \in \mathcal{A}} Y$. □

For further reference, we mention one more condition which one might impose on a finitely accessible additive category. Namely, it is well known that for a ring R, the category Flat-R is closed under products if and only if R is left coherent. This generalizes in a natural way for finitely accessible additive categories. Let us recall that an additive category $\mathcal{A}$ is said to have *weak cokernels* if for each morphism $X \to Y$ there is a morphism $Y \to Z$ such that $\mathcal{A}(Z, W) \to \mathcal{A}(Y, W) \to \mathcal{A}(X, W)$ is exact for all $W \in \mathcal{A}$.

Lemma 4.5. *Let $\mathcal{B}$ be a finitely accessible additive category and $\mathcal{A} = \mathrm{fp}(\mathcal{B})$. Then the following are equivalent:*

(1) *$\mathcal{B}$ has products.*
(2) Flat-$\mathcal{A}$ *is closed under products in* Mod-$\mathcal{A}$.
(3) *$\mathcal{A}$ has weak cokernels.*

Proof. See [8, §2.1]. □

Remark. If $\mathcal{B}$ has products, one can give a more classical proof for Proposition 4.4. Namely, one can then replace the argument by Guil Asensio, Izurdiaga and Torrecillas [13] by an older and simpler argument by Chase [7, Theorem 3.1].

5. When is the homotopy category well generated?

In this final section, we have developed enough tools to answer the question when exactly is the homotopy category of complexes $\mathbf{K}(\mathcal{B})$ well generated if $\mathcal{B}$ is a finitely accessible additive category. This way, we will generalize Proposition 2.6 and also give a rather complete answer to [15, Question 4.2] asked by Holm and Jørgensen. Finally, we will give another criterion for a triangulated category to be (or not to be) well generated and this way construct other classes of examples of categories which are not well generated.
First, we recall a crucial result due to Neeman:

Lemma 5.1. *Let $\mathcal{A}$ be a skeletally small additive category. Then the homotopy category $\mathbf{K}(\text{Proj-}\mathcal{A})$ is $\aleph_1$–well generated. If, moreover, $\mathcal{A}$ has weak cokernels, then $\mathbf{K}(\text{Proj-}\mathcal{A})$ is compactly generated.*

Proof. Neeman has proved in [31, Theorem 1.1] that, given a ring R, the category $\mathbf{K}(\text{Proj-}R)$ is $\aleph_1$–well generated, and if R is left coherent then $\mathbf{K}(\text{Proj-}R)$ is even compactly generated. The actual arguments, contained in [31, §§4–7], immediately generalize to the setting of projective modules over small categories. The role of finitely generated free modules over R is taken by representable functors, and instead of the duality between the categories of left and right projective finitely generated modules we consider the duality between the idempotent completions of the categories of covariant and contravariant representable functors. □

We already know that $\mathbf{K}(\mathcal{B})$ is always locally well generated. When employing Lemma 5.1, we can show the following statement, which is one of the main results of this paper:

Theorem 5.2. *Let $\mathcal{B}$ be a finitely accessible additive category. Then the following are equivalent:*

(1) $\mathbf{K}(\mathcal{B})$ *is well generated;*
(2) $\mathbf{K}(\mathcal{B})$ *is $\aleph_1$–well generated;*
(3) $\mathcal{B}$ *is pure semisimple.*

If, moreover, $\mathcal{B}$ has products, then the conditions are further equivalent to

(4) $\mathbf{K}(\mathcal{B})$ *is compactly generated.*

Proof. (1) $\implies$ (3). If $\mathbf{K}(\mathcal{B})$ is well generated, it is in particular generated by a set of objects as a localizing subcategory of itself; see Proposition 1.2. Hence $\mathcal{B}$ is pure semisimple by Theorem 2.5.
(3) $\implies$ (2) and (4). If $\mathcal{B}$ is pure semisimple and $\mathcal{A} = \text{fp}(\mathcal{B})$, then $\mathcal{B}$ is equivalent to Flat-$\mathcal{A}$ by Proposition 4.2, and Flat-$\mathcal{A}$ = Proj-$\mathcal{A}$ by Proposition 4.4. The conclusion follows by Lemmas 5.1 and 4.5.

(2) or (4) $\implies$ (1). This is obvious. □

Remark. (1) Neeman proved in [31] more than stated in Lemma 5.1. He described a particular set of generators for $\mathbf{K}(\text{Proj-}\mathcal{A})$ satisfying conditions of Definition 1.1. Namely, $\mathbf{K}(\text{Proj-}\mathcal{A})$ is always $\aleph_1$–well generated by a representative set of bounded below complexes of finitely generated projectives. Moreover, he gave an explicit description of compact objects in $\mathbf{K}(\text{Proj-}\mathcal{A})$ in [31, 7.12].
(2) An exact characterization of when $\mathbf{K}(\mathcal{B})$ is compactly generated and thereby a complete answer to [15, Question 4.2] does not seem to be known. We have shown that this reduces to the problem when $\mathbf{K}(\text{Proj-}\mathcal{A})$ is compactly generated. A sufficient condition is given in Lemma 5.1, but it is probably not necessary. On the other hand, if $R = k[x_1, x_2, x_3, \dots]/(x_ix_j;\ i,j \in \mathbb{N})$ where k is a field, then $\mathbf{K}(\text{Flat-}R)$ coincides with $\mathbf{K}(\text{Proj-}R)$, but the latter is not a compactly generated triangulated category; see [31, 7.16] for details.

Example 5.3. The above theorem adds other locally well generated but not well generated triangulated categories to our repertoire. For example $\mathbf{K}(\mathcal{TF})$, where $\mathcal{TF}$ stands for the category of all torsion-free abelian groups, has this property.

We finish the paper with some examples of triangulated categories where the fact that they are not generated by a set is less obvious. For this purpose, we will use the following criterion:

Proposition 5.4. *Let $\mathcal{T}$ be a locally well generated triangulated category and $\mathcal{L}$ be a localizing subcategory. Consider the diagram*

$$\mathcal{L} \xrightarrow{\subseteq} \mathcal{T} \xrightarrow{Q} \mathcal{T}/\mathcal{L}.$$

If two of the categories $\mathcal{L}$, $\mathcal{T}$ and $\mathcal{T}/\mathcal{L}$ are well generated, so is the third.

Proof. If $\mathcal{L} = \operatorname{Loc}\mathcal{S}$ and $\mathcal{T}/\mathcal{L} = \operatorname{Loc}\mathcal{C}$ for some sets $\mathcal{S}, \mathcal{C}$, let $\mathcal{L}'$ be the localizing subcategory of $\mathcal{T}$ generated by the set of objects $\mathcal{S} \cup \mathcal{C}$. Lemma 3.8 yields the equality $\mathcal{T}/\mathcal{L} = \mathcal{L}'/\mathcal{L}$. Hence also $\mathcal{T} = \mathcal{L}'$, so $\mathcal{T}$ is generated by a set, and consequently $\mathcal{T}$ is well generated.
If $\mathcal{L}$ and $\mathcal{T}$ are well generated, so is $\mathcal{T}/\mathcal{L}$ by [26, 7.2.1]. Finally, one knows that $X \in \mathcal{T}$ belongs to $\mathcal{L}$ if and only if $QX = 0$; see [32, 2.1.33 and 1.6.8]. Therefore, if $\mathcal{T}$ and $\mathcal{T}/\mathcal{L}$ are well generated, so is $\mathcal{L}$ by [26, 7.4.1]. □

Remark. We stress here that by saying that $\mathcal{T}/\mathcal{L}$ is well generated, we in particular mean that $\mathcal{T}/\mathcal{L}$ is a usual category in the sense that all morphism spaces are sets and *not* proper classes.

Now we can conclude by showing that some homotopy categories of acyclic complexes are not well generated.

Example 5.5. Let R be a ring, $\mathbf{K}_{\text{ac}}(\text{Mod-}R)$ be the full subcategory of $\mathbf{K}(\text{Mod-}R)$ formed by all acyclic complexes, and $\mathcal{L} = \operatorname{Loc}\{R\}$. It is well-known but also an easy consequence of Proposition 3.6 that the composition

$$\mathbf{K}_{\text{ac}}(\text{Mod-}R) \xrightarrow{\subseteq} \mathbf{K}(\text{Mod-}R) \xrightarrow{Q} \mathbf{K}(\text{Mod-}R)/\mathcal{L}$$

is a triangle equivalence between $\mathbf{K}(\text{Mod-}R)/\mathcal{L}$ and $\mathbf{K}_{\text{ac}}(\text{Mod-}R)$.
By Proposition 2.6, $\mathbf{K}(\text{Mod-}R)$ is well generated if and only if R is right pure semisimple. Therefore, $\mathbf{K}_{\text{ac}}(\text{Mod-}R)$ is well generated if and only if R is right pure semisimple by Proposition 5.4. In fact, $\mathbf{K}_{\text{ac}}(\text{Mod-}R)$ is not generated by any set of objects if R is not right pure semisimple. As particular examples, we may take $R = \mathbb{Z}$ or $R = k(\cdot \rightrightarrows \cdot)$ for any field k.

Example 5.6. Let $\mathcal{B}$ be a finitely accessible category. Recall that $\mathcal{B}$ is equivalent to Flat-$\mathcal{A}$ for $\mathcal{A} = \text{fp}(\mathcal{B})$. Then the natural exact structure on Flat-$\mathcal{A}$ coming from Mod-$\mathcal{A}$ is nothing else than the well-known exact structure given by pure exact short sequences in $\mathcal{B}$ (see eg. [8]).
We denote by $\mathbf{K}_{\text{pac}}(\text{Flat-}\mathcal{A})$ the full subcategory of $\mathbf{K}(\text{Flat-}\mathcal{A})$ formed by all complexes exact with respect to this exact structure, and call such complexes *pure acyclic*. More explicitly, $X \in \mathbf{K}(\text{Flat-}\mathcal{A})$ is pure acyclic if and only if X is acyclic in Mod-$\mathcal{A}$ and all the cycles $Z^i(X)$ are flat. Note that $\mathbf{K}_{\text{pac}}(\text{Flat-}\mathcal{A})$ is closed under taking coproducts in $\mathbf{K}(\text{Flat-}\mathcal{A})$.
Neeman proved in [31, Theorem 8.6] that $X \in \mathbf{K}(\text{Flat-}\mathcal{A})$ is pure acyclic if and only if there are no non-zero homomorphisms from any $Y \in \mathbf{K}(\text{Proj-}\mathcal{A})$ to X. Then either by combining Proposition 3.6 with Lemma 5.1 or by using [31, 8.1 and 8.2], one shows that the composition

$$\mathbf{K}_{\text{pac}}(\text{Flat-}\mathcal{A}) \xrightarrow{\subseteq} \mathbf{K}(\text{Flat-}\mathcal{A}) \xrightarrow{Q} \mathbf{K}(\text{Flat-}\mathcal{A})/\mathbf{K}(\text{Proj-}\mathcal{A})$$

is a triangle equivalence. Now again, Proposition 5.4 implies that $\mathbf{K}_{\text{pac}}(\text{Flat-}\mathcal{A})$ is well generated if and only if $\mathcal{B}$ is pure semisimple. If $\mathcal{B}$ is of the form Flat-R for a ring R, this precisely means that R is right perfect.
As a particular example, $\mathbf{K}_{\text{pac}}(\mathcal{TF})$ is locally well generated but not well generated, where $\mathcal{TF}$ stands for the class of all torsion-free abelian groups.

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Semigroup Properties for the Second Fundamental Form

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Abstract. Let M be a compact Riemannian manifold with boundary ∂M and $L=\delta+Z$ for a C^1-vector field Z on M. Several equivalent statements, including the gradient and Poincaré/log-Sobolev type inequalities of the Neumann semigroup generated by L, are presented for lower bound conditions on the curvature of L and the second fundamental form of ∂M. The main result not only generalizes the corresponding known ones on manifolds without boundary, but also clarifies the role of the second fundamental form in the analysis of the Neumann semigroup. Moreover, the Lévy-Gromov isoperimetric inequality is also studied on manifolds with boundary.

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1 Introduction

The main purpose of this paper is to find out equivalent properties of the Neumann semigroup on manifolds with boundary for lower bounds of the second fundamental form of the boundary. To explain the main idea of the study, let us briefly recall some equivalent semigroup properties for curvature lower bounds on manifolds without boundary.
Let M be a connected complete Riemannian manifold without boundary and let $L=\Delta+Z$ for some C^1-vector field Z on M. Let P_t be the diffusion semigroup generated by L, which is unique and Markovian if the curvature of L is bounded below, namely (see [3]),

$$\mathrm{Ric}-\nabla Z\geq -K \tag{1.1}$$

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holds on M for some constant $K \in \mathbb{R}$. The following is a collection of known equivalent statements for (1.1), where the first two ones on gradient estimates are classical in geometry (see e.g. [1, 5, 6, 7]), and the remainder follows from Propositions 2.1 and 2.6 in [2] (see also [9]):

(i) $|\nabla P_t f|^2 \le e^{2Kt} P_t |\nabla f|^2, \quad t \ge 0, \ f \in C_b^1(M)$;

(ii) $|\nabla P_t f| \le e^{Kt} P_t |\nabla f|, \quad t \ge 0, \ f \in C_b^1(M)$;

(iii) $P_t f^2 - (P_t f)^2 \le \dfrac{e^{2Kt}-1}{K} P_t |\nabla f|^2, \quad t \ge 0, \ f \in C_b^1(M)$;

(iv) $P_t f^2 - (P_t f)^2 \ge \dfrac{1-e^{-2Kt}}{K} |\nabla P_t f|^2, \quad t \ge 0, \ f \in C_b^1(M)$;

(v) $P_t(f^2 \log f^2) - (P_t f^2)\log(P_t f^2) \le \dfrac{2(e^{2Kt}-1)}{K} P_t |\nabla f|^2, \quad t \ge 0, \ f \in C_b^1(M)$;

(vi) $(P_t f)\{P_t(f \log f) - (P_t f)\log(P_t f)\} \ge \dfrac{1-e^{-2Kt}}{2K} |\nabla P_t f|^2, \quad t \ge 0, \ f \in C_b^1(M), \ f \ge 0$.

These equivalent statements for the curvature condition are crucial in the study of heat semigroups and functional inequalities on manifolds. For the case that M has a convex boundary, these equivalences are also true for P_t the Neumann semigroup (see [10] for one more equivalent statement on Harnack inequality). The question is now can we extend this result to manifolds with non-convex boundary, and furthermore describe the second fundamental using semigroup properties?

So, from now on we assume that M has a boundary ∂M. Let N be the inward unit normal vector field on ∂M. Then the second fundamental form is a two-tensor on $T\partial M$, the tangent space of ∂M, defined by

$$\mathbb{I}(X,Y) = -\langle \nabla_X N, Y\rangle, \quad X, Y \in T\partial M.$$

If $\mathbb{I} \ge 0$(i.e. $\mathbb{I}(X,X) \ge 0$ for $X \in T\partial M$), then ∂M (or M) is called convex. In general, we intend to study the lower bound condition of $\mathbb{I}$; namely, $\mathbb{I} \ge -\sigma$ on ∂M for some $\sigma \in \mathbb{R}$.

For $x \in M$, let $\mathbb{E}^x$ be the expectation taken for the reflecting L-diffusion process X_t starting from x. So, for a bounded measurable functional Φ of X,

$$\mathbb{E}\Phi : \ x \mapsto \mathbb{E}^x \Phi$$

is a function on M. Moreover, let l_t be the local time of X_t on ∂M. According to [8, Theorem 5.1], (1.1) and $\mathbb{I} \ge -\sigma$ imply

$$|\nabla P_t f| \le e^{Kt} \mathbb{E}\big[|\nabla f|(X_t)|e^{\sigma l_t}\big], \quad t > 0, f \in C^1(M). \tag{1.2}$$

To see that (1.2) is indeed equivalent to (1.1) and $\mathbb{I} \geq -\sigma$, we shall make use of the following formula for the second fundamental form established recently by the author in [12]: for any $f \in C^\infty(M)$ satisfying the Neumann condition $Nf|_{\partial M} = 0$,

$$\mathbb{I}(\nabla f, \nabla f) = \frac{\sqrt{\pi}|\nabla f|^2}{2} \lim_{t\to 0} \frac{1}{\sqrt{t}} \log \frac{(P_t|\nabla f|^p)^{1/p}}{|\nabla P_t f|} \tag{1.3}$$

holds on ∂M for any $p \in [1, \infty)$. With help of this result and stochastic analysis on the reflecting diffusion process, we are able to prove the following main result of the paper.

Theorem 1.1. *Let M be a compact Riemannian manifold with boundary and let P_t be the Neumann semigroup generated by $L = \Delta + Z$. Then for any constants $K, \sigma \in \mathbb{R}$, the following statements are equivalent to each other:*

(1) $\mathrm{Ric} - \nabla Z \geq -K$ *on* M *and* $\mathbb{I} \geq -\sigma$ *on* ∂M*;*

(2) (1.2) *holds;*

(3) $|\nabla P_t f|^2 \leq \mathrm{e}^{2Kt}(P_t|\nabla f|^2)\mathbb{E}\mathrm{e}^{2\sigma l_t}, \quad t \geq 0,\ f \in C^1(M)$;

(4) $P_t(f^2 \log f^2) - (P_t f^2) \log P_t f^2 \leq 4\mathbb{E}\big[|\nabla f|^2(X_t) \int_0^t \mathrm{e}^{2\sigma(l_t - l_{t-s}) + 2Ks}\mathrm{d}s\big]$, $t \geq 0,\ f \in C^1(M)$;

(5) $P_t f^2 - (P_t f)^2 \leq 2\mathbb{E}\big[|\nabla f|^2(X_t) \int_0^t \mathrm{e}^{2\sigma(l_t - l_{t-s}) + 2Ks}\mathrm{d}s\big],\ t \geq 0,\ f \in C^1(M)$;

(6) $|\nabla P_t f|^2 \leq$
$\leq \Big(\frac{2K}{1 - \mathrm{e}^{-2Kt}}\Big)^2 \big(P_t(f \log f) - (P_t f) \log P_t f\big)\mathbb{E}\big[f(X_t) \int_0^t \mathrm{e}^{2\sigma l_s - 2Ks}\mathrm{d}s\big]$,
$t > 0,\ f \geq 0,\ f \in C^1(M)$;

(7) $|\nabla P_t f|^2 \leq \dfrac{2K^2}{(1 - \mathrm{e}^{-2Kt})^2}\big(P_t f^2 - (P_t f)^2\big)\mathbb{E} \int_0^t \mathrm{e}^{2\sigma l_s - 2Ks}\mathrm{d}s, \quad t \geq 0,\ f \in C^1(M)$.

Theorem 1.1 can be extended to a class of non-compact manifolds with boundary such that the local times l_t is exponentially integrable. According to [13] the later is true provided $\mathbb{I}$ is bounded, the sectional curvature around ∂M is bounded above, the drift Z is bounded around ∂M, and the injectivity radius of the boundary is positive. To avoid technical complications, here we simply consider the compact case.

In the next section, we shall provide a result on gradient estimate and non-constant lower bounds of curvature and second fundamental form, which implies the equivalences among (1), (2) and (3) as a special case. Then we present a complete proof for the remainder of Theorem 1.1 in Section 3. As mentioned above, for manifolds without boundary or with a convex boundary an equivalent Harnack inequality for the curvature condition has been presented in [10].

Due to unboundedness of the local time which causes an essential difficulty in the study of Harnack inequality, the corresponding result for lower bound conditions of the curvature and the second fundamental form is still open. Nevertheless, log-Harnack and Harnack inequalities for the Neumann semigroup on non-convex manifolds have been provided by [13, Theorem 5.1] and [14, Theorem 4.1] respectively. Finally, as an extension to a result in [4] where manifolds without boundary is considered, the Lévy-Gromov isoperimetric inequality is derived in Section 4 for manifolds with boundary.

2 Gradient estimate

Let $K_1, K_2 \in C(M)$ be such that

$$\mathrm{Ric} - \nabla Z \geq -K_1 \text{ on } M, \quad \mathbb{I} \geq -K_2 \text{ on } \partial M. \tag{2.1}$$

According to [8, Theorem 5.1] this condition implies

$$|\nabla P_t f| \leq \mathbb{E}\big[|\nabla f|(X_t)\mathrm{e}^{\int_0^t K_1(X_s)\mathrm{d}s + \int_0^t K_2(X_s)\mathrm{d}l_s}\big], \quad t \geq 0, f \in C^1(M). \tag{2.2}$$

The main purpose of this section is to prove that these two statements are indeed equivalent to each other. To prove that (2.2) implies (2.1), we need the following results collected from [11, Proof of Lemma 2.1] and [13, Theorem 2.1, Lemma 2.2, Proposition A.2] respectively:

(I) For any $\lambda > 0$, $\mathbb{E}\mathrm{e}^{\lambda l_t} < \infty$.

(II) For $X_0 = x \in \partial M$, $\limsup_{t\to 0} \frac{1}{t}|\mathbb{E} l_t - 2\sqrt{t/\pi}| < \infty$.

(III) For $X_0 = x \in \partial M$, there exists a constant $c > 0$ such that $\mathbb{E} l_t^2 \leq ct, \quad t \in [0,1]$.

(IV) Let ρ be the Riemannian distance. For $\delta > 0$ and $X_0 = x \in M \setminus \partial M$ such that $\rho(x, \partial M) \geq \delta$, the stopping time $\tau_\delta := \inf\{t > 0 : \rho(X_t, x) \geq \delta\}$ satisfies $\mathbb{P}(\tau_\delta \leq t) \leq c\exp[-\delta^2/(16t)]$ for some constant $c > 0$ and all $t > 0$.

Theorem 2.1. (2.1), (2.2) *and the following inequality are equivalent to each other:*

$$|\nabla P_t f|^2 \leq (P_t|\nabla f|^2)\mathbb{E}\big[\mathrm{e}^{2\int_0^t K_1(X_s)\mathrm{d}s + 2\int_0^t K_2(X_s)\mathrm{d}l_s}\big], \quad t \geq 0, f \in C^1(M). \tag{2.3}$$

Proof. Since by [8] (2.1) implies (2.2) which is stronger than (2.3) due to the Schwartz inequality, it remains to deduce (2.1) from (2.3).

(a) Proof of $\mathrm{Ric} - \nabla Z \geq -K_1$. It suffices to prove at points in the interior. Let $X_0 = x \in M \setminus \partial M$. For any $\varepsilon > 0$ there exists $\delta > 0$ such that

$$\bar{B}(x,\delta) \subset M \setminus \partial M, \qquad \sup_{y\in\bar{B}(x,\delta)} |K_1(y) - K_1(x)| \le \varepsilon, \tag{2.4}$$

where $\bar{B}(x,\delta)$ is the closed geodesic ball at x with radius δ. Since $l_t = 0$ for $t \le \tau_\delta$, by (2.3), (I) and (IV) we have

$$\begin{aligned}|\nabla P_t f|^2(x) &\le (P_t|\nabla f|^2(x))\mathbb{E}\mathrm{e}^{2\int_0^t K_1(X_s)\mathrm{d}s + 2\int_0^t K_2(X_s)\mathrm{d}l_s}\\ &\le (P_t|\nabla f|^2(x))\Big\{\mathrm{e}^{2t(K_1(x)+\varepsilon)}\mathbb{P}(\tau_\delta \ge t) + \sqrt{\mathbb{P}(\tau_\delta < t)\mathbb{E}\mathrm{e}^{4t\|K_1\|_\infty + 4\|K_2\|_\infty l_t}}\Big\}\\ &\le (P_t|\nabla f|^2(x))\mathrm{e}^{2t(K_1(x)+\varepsilon)} + C\mathrm{e}^{-\lambda/t}, \quad t\in(0,1]\end{aligned}$$

for some constants $C, \lambda > 0$.
This implies

$$\limsup_{t\to0}\frac{|\nabla P_t f|^2(x) - |\nabla f|^2(x)}{t} \le \limsup_{t\to0}\frac{\mathrm{e}^{2t(K_1(x)+\varepsilon)}P_t|\nabla f|^2(x) - |\nabla f|^2(x)}{t}. \tag{2.5}$$

Now, let $f\in C^\infty(M)$ with $Nf|_{\partial M} = 0$, we have

$$P_t f = f + \int_0^t P_s Lf \mathrm{d}s, \quad t \ge 0.$$

Then

$$\begin{aligned}&\limsup_{t\to0}\frac{|\nabla P_t f|^2(x) - |\nabla f|^2(x)}{t}\\ &= \lim_{t\to0}\frac{1}{t}\Big\{\Big|\int_0^t \nabla P_s Lf\mathrm{d}s\Big|^2 + 2\int_0^t\langle\nabla f, \nabla P_s Lf\rangle\mathrm{d}s\Big\}(x).\end{aligned} \tag{2.6}$$

Moreover, according to the last display in the proof of [8, Theorem 5.1] (the initial data $u_0\in O_x(M)$ was missed in the right hand side therein),

$$\nabla P_t Lf = u_0\mathbb{E}\big[M_t u_t^{-1}\nabla Lf(X_t)\big],$$

where u_t is the horizontal lift of X_t on the frame bundle $O(M)$, and M_t is a $d\times d$-matrices valued right continuous process satisfying $M_0 = I$ and (see [8, Corollary 3.6])

$$\|M_t\| \le \exp\big[\|K_1\|_\infty t + \|K_2\|_\infty l_t\big].$$

So, due to (I), $|\nabla P_\cdot Lf|$ is bounded on $[0,1]\times M$ and $\nabla P_s Lf \to \nabla Lf$ as $s\to0$. Combining this with (2.6) we obtain

$$\limsup_{t\to0}\frac{|\nabla P_t f|^2(x) - |\nabla f|^2(x)}{t} = 2\langle\nabla f, \nabla Lf\rangle(x). \tag{2.7}$$

On the other hand, applying the Itô formula to $|\nabla f|^2(X_t)$ we have

$$\begin{aligned} P_t|\nabla f|^2(x) &= |\nabla f|^2(x) + \int_0^t P_s L|\nabla f|^2(x)\mathrm{d}s + \mathbb{E}\int_0^t N|\nabla f|^2(X_s)\mathrm{d}l_s \\ &\le |\nabla f|^2(x) + \int_0^t P_s L|\nabla f|^2(x)\mathrm{d}s + \|\nabla|\nabla f|^2\|_\infty \mathbb{E}l_t. \end{aligned} \tag{2.8}$$

Since $l_t = 0$ for $t \le \tau_\delta$, by (III) and (IV) we have

$$\mathbb{E}l_t \le \sqrt{(\mathbb{E}l_t^2)\mathbb{P}(\tau_\delta \le t)} \le c_1 \mathrm{e}^{-\lambda/t}, \quad t \in (0,1]$$

for some constants $c_1, \lambda > 0$. So, it follows from (2.8) that

$$\limsup_{t\to 0} \frac{P_t|\nabla f|^2(x) - |\nabla f|^2(x)}{t} \le L|\nabla f|^2(x).$$

Combining this with (2.5) and (2.7), we arrive at

$$\frac{1}{2}L|\nabla f|^2(x) - \langle \nabla f, \nabla Lf\rangle(x) \ge -(K_1(x)+\varepsilon), \quad f \in C^\infty(M), Nf|_{\partial M} = 0.$$

According to the Bochner-Weitzenböck formula, this is equivalent to $(\mathrm{Ric} - \nabla Z)(x) \ge -(K_1(x)+\varepsilon)$. Therefore, $\mathrm{Ric} - \nabla Z \ge -K_1$ holds on M by the arbitrariness of $x \in M \setminus \partial M$ and $\varepsilon > 0$.

(b) Proof of $\mathbb{I} \ge -K_2$. Let $X_0 = x \in \partial M$. For any $f \in C^\infty(M)$ with $Nf|_{\partial M} = 0$, (2.3) implies that

$$|\nabla P_t f|^2(x) \le \mathrm{e}^{C_1 t}(P_t|\nabla f|^2(x))\mathbb{E}\mathrm{e}^{2\int_0^t K_2(X_s)\mathrm{d}l_s}, \tag{2.9}$$

where $C_1 = 2\|K_1\|_\infty$. Let

$$\varepsilon_t = 2\sup_{s\in[0,t]} |K_2(X_s) - K_2(x)|.$$

By the continuity of the reflecting diffusion process we have $\varepsilon_t \downarrow 0$ as $t \downarrow 0$. Since there exists $c_0 > 0$ such that for any $r \ge 0$ one has $\mathrm{e}^r \le 1 + r + c_0 r^{3/2}\mathrm{e}^r$, we obtain

$$\log \mathbb{E}\mathrm{e}^{2\int_0^t K_2(X_s)\mathrm{d}l_s} \le \log\left\{1 + 2K_2(x)\mathbb{E}l_t + \mathbb{E}(\varepsilon_t l_t) + C_2\mathbb{E}(l_t^{3/2}\mathrm{e}^{C_2 l_t})\right\} \tag{2.10}$$

for some constant $C_2 > 0$. Moreover, by (I) and (III) we have

$$\mathbb{E}(l_t^{3/2}\mathrm{e}^{C_2 l_t}) \le (\mathbb{E}l_t^2)^{3/4}(\mathbb{E}\mathrm{e}^{4C_2 l_t})^{1/4} \le C_3 t^{3/4}, \quad t \in (0,1]$$

for some constant $C_3 > 0$. Substituting this and (2.10) into (2.9), we arrive at

$$\limsup_{t\to 0}\frac{1}{\sqrt{t}}\log\frac{|\nabla P_t f|^2(x)}{P_t|\nabla f|^2(x)}\le \limsup_{t\to 0}\frac{2K_2(x)\mathbb{E}l_t+\mathbb{E}(\varepsilon_t l_t)}{\sqrt{t}}.$$

Since $\mathbb{E}\varepsilon_t^2\to 0$ as $t\to 0$ and $\mathbb{E}l_t^2\le ct$ due to (III), this and (II) imply

$$\limsup_{t\to 0}\frac{1}{\sqrt{t}}\log\frac{|\nabla P_t f|^2(x)}{P_t|\nabla f|^2(x)}\le \frac{4K_2(x)}{\sqrt{\pi}}.$$

Combining this with (1.3) for $p=2$ we complete the proof. □

3 Proof of Theorem 1.1

Applying Theorem 2.1 to $K_1=K$ and $K_2=\sigma$ we conclude that (1), (2) and (3) are equivalent to each other. Noting that the log-Sobolev inequality (4) implies the Poincaré inequality (5) (see e.g. [6]), it suffices to prove that (2) ⇒ (4), (5) ⇒ (1), and (2) ⇒ (6) ⇒ (7) ⇒ (1), where " ⇒" stands for "implies". We shall complete the proof step by step.

(a) (2) ⇒ (4). By approximations we may assume that $f\in C^\infty(M)$ with $Nf|_{\partial M}=0$. In this case

$$\frac{\mathrm{d}}{\mathrm{d}t}P_t f = LP_t f = P_t Lf.$$

So, for fixed $t>0$ it follows from (2) that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}P_{t-s}\{(P_s f^2)\log P_s f^2\} &= -P_{t-s}\frac{|\nabla P_s f^2|^2}{P_s f^2}\\ &\ge -4\mathrm{e}^{2Ks}P_{t-s}\frac{(\mathbb{E}[f|\nabla f|(X_s)\mathrm{e}^{\sigma l_s}])^2}{P_s f^2}\\ &\ge -4\mathrm{e}^{2Ks}P_{t-s}\mathbb{E}[|\nabla f|^2(X_s)\mathrm{e}^{2\sigma l_s}].\end{aligned}\tag{3.1}$$

Next, by the Markov property, for $\mathscr{F}_s=\sigma(X_r:r\le s), s\ge 0$, we have

$$\begin{aligned}P_{t-s}(\mathbb{E}[|\nabla f|^2(X_s)\mathrm{e}^{2\sigma l_s}])(x) &= \mathbb{E}^x\mathbb{E}^{X_{t-s}}[|\nabla f|^2(X_s)\mathrm{e}^{2\sigma l_s}]\\ &= \mathbb{E}^x[\mathbb{E}^x(\mathrm{e}^{2\sigma(l_t-l_{t-s})}|\nabla f|^2(X_t)|\mathscr{F}_{t-s})]\\ &= \mathbb{E}^x[|\nabla f|^2(X_t)\mathrm{e}^{2\sigma(l_t-l_{t-s})}].\end{aligned}$$

Combining this with (3.1) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}s}P_{t-s}\{(P_s f^2)\log P_s f^2\}\ge -4\mathbb{E}\big[|\nabla f|^2(X_t)\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}\big],\quad s\in(0,t).$$

This implies (4) by integrating both sides with respect to ds from 0 to t.

(b1) (5) $\Rightarrow$ $\mathrm{Ric}-\nabla Z\geq -K$. Let $X_0=x\in M\setminus\partial M$ and $f\in C^\infty(M)$ with $Nf|_{\partial M}=0$. By (5) we have

$$P_tf^2-(P_tf)^2\leq 2\mathbb{E}\bigg[|\nabla f|^2(X_t)\int_0^t \mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}\mathrm{d}s\bigg]. \tag{3.2}$$

Let $\delta>0$ and τ_δ be as in the proof of Theorem 2.1(a). Then

$$\begin{aligned}&\mathbb{E}\bigg[|\nabla f|^2(X_t)\int_0^t \mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}\mathrm{d}s\bigg]\\&\leq (P_t|\nabla f|^2)\int_0^t\mathrm{e}^{2Ks}\mathrm{d}s+t\|\nabla f\|_\infty \mathrm{e}^{2Kt}\mathbb{E}[\mathrm{e}^{2\sigma l_t}1_{\{\tau_\delta<t\}}]\\&\leq\frac{\mathrm{e}^{2Kt}-1}{2K}P_t|\nabla f|^2(x)+c\mathrm{e}^{-\lambda/t},\quad t\in(0,1]\end{aligned}$$

holds for some constants $c,\lambda>0$ according to (IV). Combining this with (3.2) we conclude that

$$P_tf^2(x)-(P_tf)^2(x)\leq\frac{\mathrm{e}^{2Kt}-1}{K}P_t|\nabla f|^2(x)+2c\mathrm{e}^{-\lambda/t},\quad t\in(0,1]. \tag{3.3}$$

Since $f\in C^\infty(M)$ with $Nf|_{\partial M=0}$, we have

$$\begin{aligned}P_tf^2-(P_tf)^2&=f^2+\int_0^t P_sLf^2\mathrm{d}s-\Big(f+\int_0^t P_sLf\mathrm{d}s\Big)^2\\&=\int_0^t(P_sLf^2-2fP_sLf)\mathrm{d}s-\Big(\int_0^t P_sLf\mathrm{d}s\Big)^2.\end{aligned} \tag{3.4}$$

Moreover, by the continuity of $s\mapsto P_sLf$, we have

$$\Big(\int_0^t P_sLf\mathrm{d}s\Big)^2=(Lf)^2t^2+\circ(t^2), \tag{3.5}$$

where and in what follows, for a positive function $(0,1]\ni t\mapsto\xi_t$ the notion $\circ(\xi_t)$ stands for a variable such that $\circ(\xi_t)/\xi_t\to 0$ as $t\to 0$; while $\bigcirc(\xi_t)$ satisfies that $\bigcirc(\xi_t)/\xi_t$ is bounded for $t\in(0,1]$. Moreover, since

$$\begin{aligned}P_sLf^2-2fP_sLf=&Lf^2-2fLf+\int_0^s(P_rL^2f^2-2fP_rL^2f)\mathrm{d}r\\&+\mathbb{E}\int_0^s(NLf^2-2f(x)NLf)(X_r)\mathrm{d}l_r,\end{aligned}$$

and due to (IV)

$$\left|\mathbb{E}\int_0^t \big\{NLf^2 - 2f(x)NLf\big\}(X_r)\mathrm{d}l_r\right| \le c_1\mathbb{E}l_s \le c_2 \mathrm{e}^{-\lambda/s}, \quad s\in(0,1]$$

holds for some constants $c_1, c_2, \lambda > 0$, it follows from the continuity of P_s in s that

$$\int_0^t (P_sLf^2 - 2fP_sLf)\mathrm{d}s = 2t|\nabla f|^2 + \frac{t^2}{2}(L^2f^2 - 2fL^2f) + \circ(t^2).$$

Combining this with (3.4) and (3.5) we obtain

$$\begin{aligned} P_tf^2(x) - (P_tf)^2(x) &= \\ &= 2t|\nabla f|^2(x) + \frac{t^2}{2}(L^2f^2 - 2fL^2f)(x) - t^2(Lf)^2(x) + \circ(t^2) \\ &= 2t|\nabla f|^2(x) + t^2(2\langle\nabla f, \nabla Lf\rangle + L|\nabla f|^2)(x) + \circ(t^2). \end{aligned} \tag{3.6}$$

Similarly,

$$\begin{aligned} P_t|\nabla f|^2(x) &= |\nabla f|^2(x) + \int_0^t P_sL|\nabla f|^2(x)\mathrm{d}s + \mathbb{E}\int_0^t N|\nabla f|^2(X_s)\mathrm{d}l_s \\ &= |\nabla f|^2(x) + tL|\nabla f|^2(x) + \circ(t). \end{aligned}$$

Combining this with (3.3) and (3.6) we arrive at

$$\begin{aligned} &\frac{1}{t^2}\big\{t^2(2\langle\nabla f, \nabla Lf\rangle + L|\nabla f|^2)(x) + \circ(t^2)\big\} \\ &\le \frac{\mathrm{e}^{2Kt}-1}{Kt}L|\nabla f|^2(x) + \circ(1) + \frac{1}{t}\Big(\frac{\mathrm{e}^{2Kt}-1}{Kt} - 2\Big)|\nabla f|^2(x). \end{aligned}$$

Letting $t \to 0$ we obtain

$$L|\nabla f|^2(x) - 2\langle\nabla f, \nabla Lf\rangle(x) \ge -2K|\nabla f|^2(x),$$

which implies $(\mathrm{Ric} - \nabla Z)(x) \ge -K$ by the Bochner-Weitzenböck formula.
(b2) (5) $\Rightarrow$ $\mathbb{I} \ge -\sigma$. Let $X_0 = x \in \partial M$ and $f \in C^\infty(M)$ with $Nf|_{\partial M} = 0$. Noting that $Lf^2 - 2fLf = 2|\nabla f|^2$, by the Itô formula we have

$$\begin{aligned} &P_tf^2(x) - (P_tf)^2(x) = f^2 + \int_0^t P_sLf^2\mathrm{d}s - \Big(f + \int_0^t P_sLf\mathrm{d}s\Big)^2 \\ &= 2\int_0^t P_s|\nabla f|^2(x)\mathrm{d}s + 2\int_0^t [P_s(fLf)(x) - f(x)P_sLf(x)]\mathrm{d}s + \bigcirc(t^2). \end{aligned} \tag{3.7}$$

Since $Nf|_{\partial M} = 0$ implies

$$0 = \langle \nabla f, \nabla \langle N, \nabla f\rangle\rangle = \mathrm{Hess}_f(N, \nabla f) - \mathbb{I}(\nabla f, \nabla f),$$

it follows that

$$\mathbb{I}(\nabla f, \nabla f) = \mathrm{Hess}_f(N, \nabla f) = \frac{1}{2} N|\nabla f|^2. \tag{3.8}$$

So, by the Itô formula, (II) and (III) yield

$$\begin{aligned} P_s|\nabla f|^2(x) &= |\nabla f|^2(x) + \int_0^s P_r L|\nabla f|^2(x)\mathrm{d}r + \mathbb{E}\int_0^s N|\nabla f|^2(X_r)\mathrm{d}l_r \\ &= |\nabla f|^2(x) + \bigcirc(s) + 2\mathbb{E}\int_0^s \mathbb{I}(\nabla f, \nabla f)(X_r)\mathrm{d}l_r \\ &= |\nabla f|^2(x) + \frac{4\sqrt{s}}{\sqrt{\pi}}\mathbb{I}(\nabla f, \nabla f)(x) + \circ(s^{1/2}). \end{aligned} \tag{3.9}$$

Moreover, since $(fNLf)(X_r) - f(x)(NLf)(X_r)$ is bounded and goes to zero as $r \to 0$, it follows from (III) that

$$2\mathbb{E}\int_0^t \mathrm{d}s \int_0^s [(fNf)(X_r) - f(x)(NLf)(X_r)]\mathrm{d}l_r = \circ(t^{3/2}).$$

So, by the Iô formula

$$\begin{aligned} &2\int_0^t [P_s(fLf)(x) - f(x)P_sLf(x)]\mathrm{d}s \\ &= 2\int_0^t \mathrm{d}s \int_0^s [P_rL(fLf)(x) - f(x)P_rL^2f(x)]\mathrm{d}r \\ &\quad + 2\mathbb{E}\int_0^t \mathrm{d}s \int_0^s [(fNLf)(X_r) - f(x)(NLf)(X_r)]\mathrm{d}l_r = \circ(t^{3/2}). \end{aligned}$$

Combining this with (3.7) and (3.9) we arrive at

$$\begin{aligned} &\lim_{t\to 0} \frac{1}{t\sqrt{t}}\big(P_tf^2(x) - (P_tf)^2(x) - 2t|\nabla f|^2(x)\big) \\ &= \frac{8}{\sqrt{\pi}}\mathbb{I}(\nabla f, \nabla f)(x) \lim_{t\to 0}\frac{1}{t\sqrt{t}}\int_0^t \sqrt{s}\,\mathrm{d}s = \frac{16}{3\sqrt{\pi}}\mathbb{I}(\nabla f, \nabla f)(x). \end{aligned} \tag{3.10}$$

On the other hand, by the Itô formula for $|\nabla f|^2(X_t)$, it follows from (3.8) and (II) that

$$\begin{aligned}
A_t &:= \\
&= \frac{1}{t\sqrt{t}}\mathbb{E}\Big\{|\nabla f|^2(X_t)\int_0^t \mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}\mathrm{d}s - t|\nabla f|^2(x)\Big\}\\
&= \frac{1}{\sqrt{t}}\big(\mathbb{E}|\nabla f|^2(X_t)-|\nabla f|^2(x)\big)+\mathbb{E}\Big\{\frac{|\nabla f|^2(X_t)}{t\sqrt{t}}\int_0^t\big(\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}-1\big)\mathrm{d}s\Big\}\\
&= \frac{1}{\sqrt{t}}\Big\{\int_0^t P_sL|\nabla f|^2(x)\mathrm{d}s+\mathbb{E}\int_0^t N|\nabla f|^2(X_s)\mathrm{d}l_s\Big\}\\
&\quad +\mathbb{E}\Big\{\frac{|\nabla f|^2(X_t)}{t\sqrt{t}}\int_0^t\big(\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}-1\big)\mathrm{d}s\Big\}\\
&= \frac{4}{\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)(x)+\circ(1)+\mathbb{E}\Big\{\frac{|\nabla f|^2(X_t)}{t\sqrt{t}}\int_0^t\big(\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}-1\big)\mathrm{d}s\Big\}.
\end{aligned} \tag{3.11}$$

Since by (I) and (III)

$$\begin{aligned}
&\Big|\mathbb{E}\Big[\big(|\nabla f|^2(X_t)-|\nabla f|^2(x)\big)\int_0^t\big(\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}-1\big)\mathrm{d}s\Big]\Big|\\
&\le t\Big\{\mathbb{E}\big(|\nabla f|^2(X_t)-|\nabla f|^2(x)\big)^2\Big\}^{1/2}\Big\{\mathbb{E}\big(\mathrm{e}^{2Kt+2\sigma l_t}-1\big)^2\Big\}^{1/2}\\
&= \circ(t)\cdot\big(\mathbb{E}[4\sigma^2 l_t^2]+\circ(t)\big)=\circ(t^2),
\end{aligned}$$

it follows from (I) and (II) that

$$\begin{aligned}
&\mathbb{E}\Big[|\nabla f|^2(X_t)\int_0^t\big(\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}-1\big)\mathrm{d}s\Big]\\
&= \circ(t^2)+|\nabla f|^2(x)\mathbb{E}\int_0^t\big(\mathrm{e}^{2Ks+2\sigma(l_t-l_{t-s})}-1\big)\mathrm{d}s\\
&= \circ(t^{3/2})+\frac{4\sigma|\nabla f|^2(x)}{\sqrt{\pi}}\int_0^t\big(\sqrt{t}-\sqrt{t-s}\big)\mathrm{d}s\\
&= \frac{4\sigma t\sqrt{t}}{3\sqrt{\pi}}|\nabla f|^2(x)+\circ(t^{3/2}).
\end{aligned}$$

Combining this with (3.11) we arrive at

$$A_t \le \circ(1)+\frac{4}{\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)(x)+\frac{4\sigma}{3\sqrt{\pi}}|\nabla f|^2(x).$$

So, (3.10) and (5) imply that

$$\frac{16}{3\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)(x)\le\limsup_{t\to 0}2A_t\le\frac{8}{\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)(x)+\frac{8\sigma}{3\sqrt{\pi}}|\nabla f|^2(x).$$

Therefore, $\mathbb{I}(\nabla f, \nabla f)(x) \geq -\sigma |\nabla f|^2(x)$.
(c) (2) $\Rightarrow$ (6). Let $f \geq 0$ be smooth satisfying the Neumann boundary condition. We have

$$\frac{\mathrm{d}}{\mathrm{d}s} P_s\big\{(P_{t-s}f)\log P_{t-s}f\big\} = P_s \frac{|\nabla P_{t-s}f|^2}{P_{t-s}f}.$$

This implies

$$P_t(f\log f) - (P_tf)\log P_tf = \int_0^t P_s \frac{|\nabla P_{t-s}f|^2}{P_{t-s}f}\mathrm{d}s. \tag{3.12}$$

On the other hand, by (2) and applying the Schwartz inequality to the probability measure $\frac{2K}{1-\exp[-2Kt]}\mathrm{e}^{-2Ks}\mathrm{d}s$ on $[0,t]$, we obtain

$$\begin{aligned}
&|\nabla P_tf|^2 = \\
&= \bigg\{\frac{2K}{1-\mathrm{e}^{-2Kt}}\int_0^t |\nabla P_s(P_{t-s}f)|\mathrm{e}^{-2Ks}\mathrm{d}s\bigg\}^2 \\
&\leq \bigg\{\frac{2K}{1-\mathrm{e}^{-2Kt}}\int_0^t E\big[|\nabla P_{t-s}f|(X_s)\mathrm{e}^{\sigma l_s - Ks}\big]\mathrm{d}s\bigg\}^2 \\
&\leq \Big(\frac{2K}{1-\mathrm{e}^{-2Kt}}\Big)^2\bigg(\mathbb{E}\int_0^t \frac{|\nabla P_{t-s}f|^2}{P_{t-s}f}(X_s)\mathrm{d}s\bigg)\int_0^t \mathbb{E}\big[P_{t-s}f(X_s)\mathrm{e}^{2\sigma l_s - 2Ks}\big]\mathrm{d}s \\
&= \Big(\frac{2K}{1-\mathrm{e}^{-2Kt}}\Big)^2\bigg(\int_0^t P_s\frac{|\nabla P_{t-s}f|^2}{P_{t-s}f}\mathrm{d}s\bigg)\int_0^t \mathbb{E}\big[P_{t-s}f(X_s)\mathrm{e}^{2\sigma l_s - 2Ks}\big]\mathrm{d}s.
\end{aligned}$$

Combining this with (3.12) and noting that the Markov property implies

$$\begin{aligned}
\mathbb{E}[P_{t-s}f(X_s)\mathrm{e}^{2\sigma l_s}] &= \mathbb{E}[(\mathbb{E}^{X_s}f(X_{t-s}))\mathrm{e}^{2\sigma l_s}] = \mathbb{E}[\mathrm{e}^{2\sigma l_s}\mathbb{E}(f(X_t)|\mathscr{F}_s)] \\
&= \mathbb{E}[\mathbb{E}(f(X_t)\mathrm{e}^{2\sigma l_s}|\mathscr{F}_s)] = \mathbb{E}[f(X_t)\mathrm{e}^{2\sigma l_s}],
\end{aligned}$$

we obtain (6).
(d) (6) $\Rightarrow$ (7). The proof is similar to the classical one for the log-Sobolev inequality to imply the Poincaré inequality. Let $f \in C^\infty(M)$. SInce M is compact, $1+\varepsilon f > 0$ for small $\varepsilon > 0$. Applying (6) to $1+\varepsilon f$ in place of f, we obtain

$$\begin{aligned}
|\nabla P_tf|^2 \leq &\frac{2K}{\varepsilon^2(1-\mathrm{e}^{-2Kt})}\big\{P_t(1+\varepsilon f)\log(1+\varepsilon f) - (1+\varepsilon P_tf)\log(1+\varepsilon P_tf)\big\} \\
&\cdot \mathbb{E}\bigg\{(1+\varepsilon f(X_t))\int_0^t \mathrm{e}^{2\sigma l_s - 2Ks}\mathrm{d}s\bigg\}.
\end{aligned} \tag{3.13}$$

Since by Taylor's expansion

$$P_t(1+\varepsilon f)\log(1+\varepsilon f)-(1+\varepsilon P_tf)\log(1+\varepsilon P_tf)=\frac{\varepsilon^2}{2}\big(P_tf^2-(P_tf)^2\big)+\circ(\varepsilon^2),$$

letting $\varepsilon\to 0$ in (3.13) we obtain (7).
(e1) (7) $\Rightarrow$ $\mathrm{Ric}-\nabla Z\ge -K$. Let $X_0=x\in M\setminus\partial M$ and $f\in C^\infty(M)$ with $Nf|_{\partial M}=0$. by (I) and (IV) we have

$$\mathbb{E}\mathrm{e}^{2\sigma l_s}=1+\mathbb{E}[\mathrm{e}^{2\sigma l_s}1_{\{\tau_\delta\le s\}}]=1+\circ(s).$$

So,

$$\mathbb{E}\int_0^t \mathrm{e}^{2\sigma l_s-2Ks}\mathrm{d}s=\frac{1-\exp[-2Kt]}{2K}+\circ(t).$$

Combining this with (3.6) and (7), we conclude that, at point x,

$$\begin{aligned}&\frac{|\nabla P_tf|^2-|\nabla f|^2}{t}\le\\&\le\frac{K}{1-\mathrm{e}^{-2Kt}}\big\{2|\nabla f|^2+t\big(2\langle\nabla f,\nabla Lf\rangle+L|\nabla f|^2\big)\big\}-\frac{|\nabla f|^2}{t}+\circ(1)\\&=\frac{1}{t}\Big(\frac{2Kt}{1-\mathrm{e}^{-2Kt}}-1\Big)|\nabla f|^2+\frac{Kt}{1-\mathrm{e}^{-2Kt}}\big(2\langle\nabla f,\nabla Lf\rangle+L|\nabla f|^2\big)+\circ(1).\end{aligned}$$

Letting $t\to 0$ and using (2.7), we obtain

$$2\langle\nabla f,\nabla Lf\rangle\le K|\nabla f|^2+\langle\nabla f,\nabla Lf\rangle+\frac12 L|\nabla f|^2$$

at point x. This implies $\mathrm{Ric}-\nabla Z\ge -K$ at this point according to the Bochner-Weitzenböck formula.
(e2) (7) $\Rightarrow$ $\mathbb{I}\ge-\sigma$. Let $X_0=x\in\partial M$ and $f\in C^\infty(M)$ with $Nf|_{\partial M}=0$. It follows from (3.10), (7) and (II) that at point x,

$$\begin{aligned}&|\nabla P_tf|^2\le\\&\le\frac{2K^2}{(1-\mathrm{e}^{-2Kt})^2}\Big(2t|\nabla f|^2+\frac{16t^{3/2}}{3\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)+\circ(t^{3/2})\Big)\Big(t+\frac{8\sigma t^{3/2}}{3\sqrt{\pi}}+\circ(t^{3/2})\Big)\\&=\frac{4K^2t^2}{(1-\mathrm{e}^{-2Kt})^2}|\nabla f|^2+\frac{4K^2t^{5/2}}{(1-\mathrm{e}^{-2Kt})^2}\Big(\frac{8}{3\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)+\frac{8\sigma}{3\sqrt{\pi}}|\nabla f|^2\Big)+\circ(t^{1/2}).\end{aligned}$$

Combining this with (2.7) we deduce at point x that

$$\begin{aligned}0&=\lim_{t\to0}\frac{1}{\sqrt{t}}\Big(|\nabla P_tf|^2-\frac{4K^2t^2}{(1-\mathrm{e}^{-2Kt})^2}|\nabla f|^2\Big)\\&\le\lim_{t\to0}\frac{4K^2t^2}{(1-\mathrm{e}^{-2Kt})^2}\Big(\frac{8}{3\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)+\frac{8\sigma}{3\sqrt{\pi}}|\nabla f|^2\Big)\\&=\frac{8}{3\sqrt{\pi}}\mathbb{I}(\nabla f,\nabla f)+\frac{8\sigma}{3\sqrt{\pi}}|\nabla f|^2.\end{aligned}$$

Therefore, $\mathbb{I}(\nabla f, \nabla f)(x) \geq -\sigma|\nabla f|^2(x)$.

4 Lévy-Gromov isoperimetric inequality

As a dimension-free version of the classical Lévy-Gromov isoperimetric inequality, it is proved in [4] that if M does not have boundary then for $V \in C^2(M)$ such that $\mathrm{Ric} - \mathrm{Hess}_V \geq R > 0$ the following inequality

$$\mathscr{U}(\mu(f)) \leq \int_M \sqrt{\mathscr{U}^2(f) + R^{-1}|\nabla f|^2}\,\mathrm{d}\mu, \tag{4.1}$$

holds for any smooth function f with values in $[0,1]$, where $\mu(\mathrm{d}x) := C(V)^{-1}\mathrm{e}^{V(x)}\mathrm{d}x$ for $C(V) = \int_M \mathrm{e}^{V(x)}\mathrm{d}x$ is a probability measure on M, and $\mathscr{U} = \varphi \circ \Phi^{-1}$ for $\Phi(r) = (2\pi)^{-1}\int_{-\infty}^r \mathrm{e}^{-s^2/2}\mathrm{d}s$ and $\varphi = \Phi'$. Since $\mathscr{U}(0) = \mathscr{U}(1) = 0$, taking $f = 1_A$ (by approximations) in (4.1) for a smooth domain $A \subset M$, we obtain the isoperimetric inequality

$$R\mathscr{U}(A) \leq \mu_\partial(\partial A), \tag{4.2}$$

where $\mu_\partial(\partial A)$ is the area of ∂A induced by μ. This inequality is crucial in the study of Gaussian type concentration of μ (see [4, 9]). Obviously, (4.1) follows from the following semigroup inequality by letting $t \to \infty$:

$$\mathscr{U}(P_t f) \leq P_t\sqrt{\mathscr{U}^2(f) + R^{-1}(1-\mathrm{e}^{-2Rt})|\nabla f|^2}. \tag{4.3}$$

In this section we aim to extend (4.3) to manifolds with boundary.
Now, let again M be compact with boundary ∂M, and let P_t be the Neumann semigroup generated by $L = \Delta + Z$. We shall prove an analogue of (4.3) for the curvature and second fundamental condition in Theorem 1.1(1).

Theorem 4.1. *Let* $\mathrm{Ric} - \nabla Z \geq -K$ *and* $\mathbb{I} \geq -\sigma$ *for some constants* $K \in \mathbb{R}$ *and* $\sigma \geq 0$. *Then for any smooth function* f *with values in* $[0,1]$,

$$\mathscr{U}(P_t f) \leq \mathbb{E}\sqrt{\mathscr{U}^2(f)(X_t) + |\nabla f|^2(X_t)\frac{(\mathrm{e}^{2Kt}-1)\mathrm{e}^{2\sigma l_t}}{K}}, \quad t \geq 0. \tag{4.4}$$

If in particular ∂M *is convex (i.e.* $\sigma = 0$*), then*

$$\mathscr{U}(P_t f) \leq P_t\sqrt{\mathscr{U}^2(f) + |\nabla f|^2(X_t)\frac{\mathrm{e}^{2Kt}-1}{K}}, \quad t \geq 0.$$

If moreover $K < 0$, *then* (4.1) *and* (4.2) *hold for* $R = -K > 0$.

Proof. It suffices to prove the first assertion. To this end, we shall use the following equivalent condition for $\mathrm{Ric} - \nabla Z \geq -K$ (see e.g. the proof of [9, (1.14)]):

$$\Gamma_2(f,f) := \frac{1}{2}L|\nabla f|^2 - \langle \nabla f, \nabla Lf\rangle \geq -K|\nabla f|^2 + \frac{|\nabla|\nabla f|^2|^2}{4|\nabla f|^2}. \tag{4.5}$$

To prove (4.4), we consider the process

$$\eta_s = \mathscr{U}^2(P_{t-s}f)(X_s) + |\nabla P_{t-s}f|^2(X_s)\frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K}, \quad s\in[0,t].$$

To apply the Itô formula for η_s, recall that X_s solves the equation

$$\mathrm{d}X_s = \sqrt{2}\, u_s \circ \mathrm{d}B_s + N(X_s)\mathrm{d}l_s,$$

where u_s is the horizontal lift of X_s and B_s is the Brownian motion on $\mathbb{R}^d$ provided M is d-dimensional. So,

$$\begin{aligned}\mathrm{d}\eta_s = {} & \sqrt{2}\Big\langle 2(\mathscr{U}\mathscr{U}')(P_{t-s}f)(X_s) + \frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K}\nabla|\nabla P_{t-s}f|^2(X_s), u_s\mathrm{d}B_s\Big\rangle \\ & + \Big\{2(\mathscr{U}'^2+\mathscr{U}\mathscr{U}'')(P_{t-s}f)|\nabla P_{t-s}f|^2 + 2\Gamma_2(P_{t-s}f,P_{t-s}f)\frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K} \\ & + 2|\nabla P_{t-s}f|^2\mathrm{e}^{2Ks+2\sigma l_s}\Big\}(X_s)\mathrm{d}s \\ & + \frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K}\big(N|\nabla P_{t-s}f|^2 + 2\sigma|\nabla P_{t-s}f|^2\big)(X_s)\mathrm{d}l_s.\end{aligned}$$

Noting that $\mathscr{U}\mathscr{U}'' = -1$ and $\sigma \geq 0$ so that $\mathrm{e}^{2\sigma l_s} \geq 1$, combining this with (3.8), $\mathbb{I} \geq -\sigma$ and (4.5), we obtain

$$\begin{aligned}\mathrm{d}\eta_s \geq {} & \sqrt{2}\Big\langle 2(\mathscr{U}\mathscr{U}')(P_{t-s}f)(X_s) + \frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K}\nabla|\nabla P_{t-s}f|^2(X_s), u_s\mathrm{d}B_s\Big\rangle \\ & + \Big\{2\mathscr{U}'^2(P_{t-s}f)|\nabla P_{t-s}f|^2 + \frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}|\nabla|\nabla P_{t-s}f|^2|^2}{2K|\nabla P_{t-s}f|^2}\Big\}(X_s)\mathrm{d}s.\end{aligned}$$

Therefore, there exists a martingale M_s for $s \in [0,t]$ such that

$$\begin{aligned}\mathrm{d}\eta_s^{1/2} = {} & \mathrm{d}M_s + \frac{\mathrm{d}\eta_s}{2\eta_s^{1/2}} - \\ & - \frac{\big|2(\mathscr{U}\mathscr{U}')(P_{t-s}f)\nabla P_{t-s}f + \frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K}\nabla|\nabla P_{t-s}f|^2\big|^2(X_s)}{4\eta_s^{3/2}} \\ = {} & \mathrm{d}M_s + \frac{1}{4\eta_s^{3/2}}B_s\mathrm{d}s,\end{aligned}$$

where

$$\begin{aligned}B_s :=&2\eta_s\Big(2\mathscr{U}'^2(P_{t-s}f)|\nabla P_{t-s}f|^2+\frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}|\nabla|\nabla P_{t-s}f|^2|^2}{2K|\nabla P_{t-s}f|^2}\Big)(X_s)\\&-\Big|2(\mathscr{U}\mathscr{U}')(P_{t-s}f)\nabla P_{t-s}f+\frac{\mathrm{e}^{2Ks}-1}{K}\mathrm{e}^{2\sigma l_s}\nabla|\nabla P_{t-s}f|^2\Big|^2(X_s)\\ \ge&\frac{(\mathrm{e}^{2Ks}-1)\mathrm{e}^{2\sigma l_s}}{K}\Big\{\frac{\mathscr{U}^2(P_{t-s}f)|\nabla|\nabla P_{t-s}f|^2|^2}{2|\nabla P_{t-s}f|^2}+4|\nabla P_{t-s}f|^4\mathscr{U}'^2(P_{t-s}f)\\&\qquad-4(\mathscr{U}\mathscr{U}')(P_{t-s}f)\langle\nabla P_{t-s}f,\nabla|\nabla P_{t-s}f|^2\rangle\Big\}(X_s)\\ \ge&0.\end{aligned}$$

So, $\eta_s^{1/2}$ is a sub-martingale on $[0,t]$. Therefore, $\mathbb{E}\eta_0^{1/2}\le\mathbb{E}\eta_t^{1/2}$, which is nothing but (4.4). □

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Frames and Finite Group Schemes over Complete Regular Local Rings

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Abstract. Let p be an odd prime. We show that the classification of p-divisible groups by Breuil windows and the classification of commutative finite flat group schemes of p-power order by Breuil modules hold over every complete regular local ring with perfect residue field of characteristic p. We set up a formalism of frames and windows with an abstract deformation theory that applies to Breuil windows.

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1 Introduction

Let R be a complete regular local ring of dimension r with perfect residue field k of odd characteristic p. Let $W(k)$ be the ring of Witt vectors of k. One can write $R = \mathfrak{S}/E\mathfrak{S}$ with

$$\mathfrak{S} = W(k)[[x_1, \ldots, x_r]]$$

such that $E \in \mathfrak{S}$ is a power series with constant term p. Let σ be the endomorphism of $\mathfrak{S}$ that extends the Frobenius automorphism of $W(k)$ by $\sigma(x_i) = x_i^p$. Following Vasiu and Zink, a *Breuil window* relative to $\mathfrak{S} \to R$ is a pair (Q, ϕ) where Q is a free $\mathfrak{S}$-module of finite rank, and where

$$\phi : Q \to Q^{(\sigma)}$$

is an $\mathfrak{S}$-linear map with cokernel annihilated by E.

Theorem 1.1. *The category of p-divisible groups over R is equivalent to the category of Breuil windows relative to $\mathfrak{S} \to R$.*

If R has characteristic p, this follows from more general results of A. de Jong [dJ]; this case is included here only for completeness. If $r = 1$ and E is an Eisenstein polynomial, Theorem 1.1 was conjectured by Breuil [Br] and proved by Kisin [K1]. When E is a deformation of an Eisenstein polynomial the result is proved in [VZ1].

Like in these cases one can deduce a classification of commutative finite flat group schemes of p-power order over R: A *Breuil module* relative to $\mathfrak{S} \to R$ is a triple (M, φ, ψ) where M is a finitely generated $\mathfrak{S}$-module annihilated by a power of p and of projective dimension at most one, and where

$$\varphi : M \to M^{(\sigma)}, \qquad \psi : M^{(\sigma)} \to M$$

are $\mathfrak{S}$-linear maps with $\varphi\psi = E$ and $\psi\varphi = E$. If R has characteristic zero, such triples are equivalent to pairs (M, φ) such that the cokernel of φ is annihilated by E.

Theorem 1.2. *The category of commutative finite flat group schemes over R annihilated by a power of p is equivalent to the category of Breuil modules relative to $\mathfrak{S} \to R$.* [1]

This result is applied in [VZ2] to the question whether abelian schemes or p-divisible groups defined over the complement of the maximal ideal in $\operatorname{Spec} R$ extend to $\operatorname{Spec} R$.

Frames and windows

To prove Theorem 1.1 we show that Breuil windows are equivalent to Dieudonné displays over R, which are equivalent to p-divisible groups over R by [Z2]; the same route is followed in [VZ1]. So the main part of this article is purely module theoretic.

We introduce a notion of frames and windows (motivated by [Z3]) which allows to formulate a deformation theory that generalises the deformation theory of Dieudonné displays developed in [Z2] and that also applies to Breuil windows. Technically the main point is the formalism of σ_1 in Definition 2.1; the central result is the lifting of windows in Theorem 3.2.

This is applied as follows. Let $\mathfrak{m}_R$ be the maximal ideal of R. For each positive integer a we consider the rings $\mathfrak{S}_a = \mathfrak{S}/(x_1, \ldots, x_r)^a\mathfrak{S}$ and $R_a = R/\mathfrak{m}_R^a$. There is an obvious notion of Breuil windows relative to $\mathfrak{S}_a \to R_a$ and a functor

$$\varkappa_a : (\text{Breuil windows relative to } \mathfrak{S}_a \to R_a) \to (\text{Dieudonné displays over } R_a).$$

Here $\varkappa_1$ is trivially an equivalence because $\mathfrak{S}_1 = W(k)$ and $R_1 = k$. The deformation theory implies that on both sides lifts from a to $a+1$ are classified by lifts of the Hodge filtration in a compatible way. Thus $\varkappa_a$ is an equivalence for all a by induction, and Theorem 1.1 follows.

[1] Recently, Theorems 1.1 and 1.2 have been extended to the case $p = 2$. See: *A relation between Dieudonné displays and crystalline Dieudonné theory* (in preparation).

Complements

There is some freedom in the choice of the Frobenius lift on $\mathfrak{S}$. Namely, let σ be a ring endomorphism of $\mathfrak{S}$ which preserves the ideal $J = (x_1, \ldots, x_r)$ and which induces the Frobenius on $\mathfrak{S}/p\mathfrak{S}$. If the endomorphism σ/p of J/J^2 is nilpotent modulo p, Theorems 1.1 and 1.2 hold without change.
All of the above equivalences of categories are compatible with the natural duality operations on both sides.
If the residue field k is not perfect, there is an analogue of Theorems 1.1 and 1.2 for connected groups. Here $p = 2$ is allowed. The ring $W(k)$ is replaced by a Cohen ring of k, and the operators ϕ and φ must be nilpotent modulo the maximal ideal of $\mathfrak{S}$.
In the first version of this article [L3] the formalism of frames was introduced only to give an alternative proof of the results of Vasiu and Zink [VZ1]. In response, they pointed out that both their and this approach apply in greater generality, e.g. in the case where $E \in \mathfrak{S}$ takes the form $E = g + p\epsilon$ such that ϵ is a unit and g divides $\sigma(g)$ for a general Frobenius lift σ as above. However, the method of loc. cit. seems not to give Theorem 1.1 completely.

All rings in this article are commutative and have a unit. All finite flat group schemes are commutative.

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2 Frames and windows

Let p be a prime. The following notion of frames and windows differs from [Z3]. Some definitions and arguments could be simplified by assuming that the relevant rings are local, which is the case in our applications, but we work in greater generality until section 4.
If S is a ring equipped with a ring endomorphism σ, for an S-module M we write $M^{(\sigma)} = S \otimes_{\sigma,S} M$, and for a σ-linear map of S-modules $g : M \to N$ we denote by $g^\sharp : M^{(\sigma)} \to N$ its linearisation, $g^\sharp(s \otimes m) = sg(m)$. If $g^\sharp$ is invertible, g is called a σ-linear isomorphism.

Definition 2.1. A frame is a quintuple

$$\mathscr{F} = (S, I, R, \sigma, \sigma_1)$$

consisting of a ring S, an ideal I of S, the quotient ring $R = S/I$, a ring endomorphism $\sigma : S \to S$, and a σ-linear map of S-modules $\sigma_1 : I \to S$, such that the following conditions hold:

i. $I + pS \subseteq \mathrm{Rad}(S)$,

ii. $\sigma(a) \equiv a^p \bmod pS$ for $a \in S$,

iii. $\sigma_1(I)$ generates S as an S-module.

We do not assume here that R is the specific ring considered in the introduction. In our examples $\sigma_1(I)$ contains the element 1.

Lemma 2.2. *For every frame $\mathscr{F}$ there is a unique element $\theta \in S$ such that $\sigma(a) = \theta\sigma_1(a)$ for $a \in I$.*

Proof. Condition iii means that the homomorphism $\sigma_1^\sharp : I^{(\sigma)} \to S$ is surjective. Let us choose $b \in I^{(\sigma)}$ such that $\sigma_1^\sharp(b) = 1$. Then necessarily $\theta = \sigma^\sharp(b)$. For $a \in I$ we compute $\sigma(a) = \sigma_1^\sharp(b)\sigma(a) = \sigma_1^\sharp(ba) = \sigma^\sharp(b)\sigma_1(a)$ as desired. □

Definition 2.3. Let $\mathscr{F}$ be a frame. A window over $\mathscr{F}$, also called an $\mathscr{F}$-window, is a quadruple

$$\mathscr{P} = (P, Q, F, F_1)$$

where P is a finitely generated projective S-module, $Q \subseteq P$ is a submodule, $F : P \to P$ and $F_1 : Q \to P$ are σ-linear map of S-modules, such that the following conditions hold:

1. There is a decomposition $P = L \oplus T$ with $Q = L \oplus IT$,
2. $F_1(ax) = \sigma_1(a)F(x)$ for $a \in I$ and $x \in P$,
3. $F_1(Q)$ generates P as an S-module.

A decomposition as in 1 is called a normal decomposition of (P, Q) or of $\mathscr{P}$.

Remark 2.4. The operator F is determined by F_1. Indeed, if $b \in I^{(\sigma)}$ satisfies $\sigma_1^\sharp(b) = 1$, then condition 2 implies that $F(x) = F_1^\sharp(bx)$ for $x \in P$. In particular we have $F(x) = \theta F_1(x)$ when x lies in Q.

Remark 2.5. Condition 1 implies that

1′. P/Q is a projective R-module.

If finitely generated projective R-modules lift to projective S-modules, necessarily finitely generated because $I \subseteq \mathrm{Rad}(S)$, condition 1 is equivalent to 1′. In all our examples, this lifting property holds because S is either local or I-adic.

Lemma 2.6. *Let $\mathscr{F}$ be a frame, let $P = L \oplus T$ be a finitely generated projective S-module, and let $Q = L \oplus IT$. The set of $\mathscr{F}$-window structures (P, Q, F, F_1) on these modules is mapped bijectively to the set of σ-linear isomorphisms*

$$\Psi : L \oplus T \to P$$

by the assignment $\Psi(l + t) = F_1(l) + F(t)$ for $l \in L$ and $t \in T$.

The triple (L, T, Ψ) is called a normal representation of (P, Q, F, F_1).

Proof. If (P, Q, F, F_1) is an $\mathscr{F}$-window, by conditions 2 and 3 of Definition 2.3 the linearisation of Ψ is surjective, thus bijective since P and $P^{(\sigma)}$ are projective S-modules of equal rank by conditions i and ii of Definition 2.1. Conversely, if Ψ is given, one gets an $\mathscr{F}$-window by $F(l+t) = \theta\Psi(l) + \Psi(t)$ and $F_1(l+at) = \Psi(l) + \sigma_1(a)\Psi(t)$ for $l \in L$, $t \in T$, and $a \in I$. □

Example. The Witt frame of a p-adic ring R is

$$\mathscr{W}_R = (W(R), I_R, R, f, f_1)$$

where $W(R)$ is the ring of p-typical Witt vectors of R, f is its Frobenius endomorphism, and $f_1 : I_R \to W(R)$ is the inverse of the Verschiebung homomorphism. Here $\theta = p$. We have $I_R \subseteq \mathrm{Rad}(W(R))$ because $W(R)$ is I_R-adic; see [Z1, Proposition 3]. Windows over $\mathscr{W}_R$ are 3n-displays over R in the sense of [Z1], called displays in [M2], which is the terminology we follow.

Functoriality

Let $\mathscr{F} = (S, I, R, \sigma, \sigma_1)$ and $\mathscr{F}' = (S', I', R', \sigma', \sigma_1')$ be frames.

Definition 2.7. A homomorphism of frames $\alpha : \mathscr{F} \to \mathscr{F}'$, also called a frame homomorphism, is a ring homomorphism $\alpha : S \to S'$ with $\alpha(I) \subseteq I'$ such that $\sigma'\alpha = \alpha\sigma$ and $\sigma_1'\alpha = u \cdot \alpha\sigma_1$ for a unit $u \in S'$. If $u = 1$, then α is called strict.

Remark 2.8. The unit u is unique because $\alpha\sigma_1(I)$ generates S' as an S'-module. We have $\alpha(\theta) = u\theta'$. If we want to specify u, we say that α is a u-homomorphism. There is a unique factorisation of α into frame homomorphisms

$$\mathscr{F} \xrightarrow{\alpha'} \mathscr{F}'' \xrightarrow{\omega} \mathscr{F}'$$

such that α' is strict and ω is an invertible u-homomorphism. Here $\mathscr{F}''$ is the u^{-1}-twist of $\mathscr{F}'$ defined as $\mathscr{F}'' = (S', I', R', \sigma', u^{-1}\sigma_1')$.

Let $\alpha : \mathscr{F} \to \mathscr{F}'$ be a u-homomorphism of frames.

Definition 2.9. Let $\mathscr{P}$ be an $\mathscr{F}$-window and let $\mathscr{P}'$ be an $\mathscr{F}'$-window. A homomorphism of windows $g : \mathscr{P} \to \mathscr{P}'$ over α, also called an α-homomorphism, is an S-linear map $g : P \to P'$ with $g(Q) \subseteq Q'$ such that $F'g = gF$ and $F_1'g = u \cdot gF_1$. A homomorphism of $\mathscr{F}$-windows is an $\mathrm{id}_{\mathscr{F}}$-homomorphism in the previous sense.

Lemma 2.10. *For each $\mathscr{F}$-window $\mathscr{P}$ there is a base change window $\alpha_*\mathscr{P}$ over $\mathscr{F}'$ together with an α-homomorphism of windows $\mathscr{P} \to \alpha_*\mathscr{P}$ that induces a bijection $\mathrm{Hom}_{\mathscr{F}'}(\alpha_*\mathscr{P}, \mathscr{P}') = \mathrm{Hom}_\alpha(\mathscr{P}, \mathscr{P}')$ for all $\mathscr{F}'$-windows $\mathscr{P}'$.*

Proof. Clearly this requirement determines $\alpha_*\mathscr{P}$ uniquely. It can be constructed explicitly as follows: If (L, T, Ψ) is a normal representation of $\mathscr{P}$, a normal representation of $\alpha_*\mathscr{P}$ is $(S' \otimes_S L, S' \otimes_S T, \Psi')$ where Ψ' is defined by $\Psi'(s' \otimes l) = u\sigma'(s') \otimes \Psi(l)$ and $\Psi'(s' \otimes t) = \sigma'(s') \otimes \Psi(t)$. □

If $\alpha_*\mathscr{P} = (P', Q', F', F_1')$, then $P' = S' \otimes_S P$, and $Q' \subseteq P'$ is the S'-submodule generated by $I'P'$ and by the image of Q.

Remark 2.11. As suggested in [VZ2], the above definitions of frames and windows can be generalised as follows. Instead of condition iii of Definition 2.1, the element θ given by Lemma 2.2 is taken as part of the data. For a u-homomorphism $\alpha : \mathscr{F} \to \mathscr{F}'$ of generalised frames in this sense it is necessary to require that $\alpha(\theta) = u\theta'$. For a window over a generalised frame the relation $F(x) = \theta F_1(x)$ of Remark 2.4 becomes part of the definition, and condition 3 of Definition 2.3 is replaced by the requirement that $F_1(Q) + F(P)$ generates P. Then the results of sections 2–4 hold for generalised frames and windows as well. Details are left to the reader.

Limits

Windows are compatible with projective limits of frames in the following sense. Assume that for each positive integer n we have a frame

$$\mathscr{F}_n = (S_n, I_n, R_n, \sigma_n, \sigma_{1n})$$

and a strict frame homomorphism $\pi_n : \mathscr{F}_{n+1} \to \mathscr{F}_n$ such that the involved maps $S_{n+1} \to S_n$ and $I_{n+1} \to I_n$ are surjective and $\operatorname{Ker}(\pi_n)$ is contained in $\operatorname{Rad}(S_{n+1})$. We obtain a frame $\varprojlim \mathscr{F}_n = (S, I, R, \sigma, \sigma_1)$ with $S = \varprojlim S_n$ etc. By definition, an $\mathscr{F}_*$-window is a system $\mathscr{P}_*$ of $\mathscr{F}_n$-windows $\mathscr{P}_n$ together with isomorphisms $\pi_{n*}\mathscr{F}_{n+1} \cong \mathscr{F}_n$.

Lemma 2.12. *The category of* $(\varprojlim \mathscr{F}_n)$*-windows is equivalent to the category of* $\mathscr{F}_*$*-windows.*

Proof. The obvious functor from $(\varprojlim \mathscr{F}_n)$-windows to $\mathscr{F}_*$-windows is fully faithful. We have to show that for an $\mathscr{F}_*$-window $\mathscr{P}_*$, the projective limit $\varprojlim \mathscr{P}_n = (P, Q, F, F_1)$ defined by $P = \varprojlim P_n$ etc. is a window over $\varprojlim \mathscr{F}_n$. The condition $\operatorname{Ker}(\pi_n) \subseteq \operatorname{Rad}(S_{n+1})$ implies that P is a finitely generated projective S-module and that P/Q is projective over R. In order that P has a normal decomposition it suffices to show that each normal decomposition of $\mathscr{P}_n$ lifts to a normal decomposition of $\mathscr{P}_{n+1}$. Assume that $P_n = L_n' \oplus T_n'$ and $P_{n+1} = L_{n+1} \oplus T_{n+1}$ are normal decompositions and let $P_n = L_n \oplus T_n$ be induced by the second. Since $T_n \otimes R_n \cong P_n/Q_n \cong T_n' \otimes R_n$ and $L_n \otimes R_n \cong Q_n/IP_n \cong L_n' \otimes R_n$, we have $T_n \cong T_n'$ and $L_n \cong L_n'$. Hence the two decompositions of P_n differ by an automorphism of $L_n \oplus T_n$ of the type $\omega = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ with $c : L_n \to I_nT_n$. Now ω lifts to an endomorphism $\omega' = \left(\begin{smallmatrix} a' & b' \\ c' & d' \end{smallmatrix}\right)$ of $L_{n+1} \oplus T_{n+1}$ with $c' : L_{n+1} \to I_{n+1}T_{n+1}$, and ω' is an automorphism since $\operatorname{Ker}(\pi_n) \subseteq \operatorname{Rad}(S_{n+1})$. The required lifting of normal decompositions follows. All remaining window axioms for $\varprojlim \mathscr{P}_n$ are easily checked. □

Remark 2.13. Assume that S_1 is a local ring. Then all S_n and S are local too. Hence $\varprojlim \mathscr{F}_n$ satisfies the lifting property of Remark 2.5, so the normal decomposition of P in the preceding proof is automatic.

Duality

Let $\mathscr{P}$, $\mathscr{P}'$, and $\mathscr{P}''$ be windows over a frame $\mathscr{F}$. A bilinear form of $\mathscr{F}$-windows $\beta : \mathscr{P} \times \mathscr{P}' \to \mathscr{P}''$ is an S-bilinear map $\beta : P \times P' \to P''$ such that $\beta(Q \times Q') \subseteq Q''$ and

$$\beta(F_1(x), F_1'(x')) = F_1''(\beta(x, x')) \tag{2.1}$$

for $x \in Q$ and $x' \in Q'$. Let $\mathscr{F}$ also denote the $\mathscr{F}$-window (S, I, σ, σ_1). For every $\mathscr{F}$-window $\mathscr{P}$ there is a unique dual $\mathscr{F}$-window $\mathscr{P}^t$ together with a bilinear form $\mathscr{P} \times \mathscr{P}^t \to \mathscr{F}$ which induces for each $\mathscr{F}$-window $\mathscr{P}'$ an isomorphism $\operatorname{Hom}(\mathscr{P}', \mathscr{P}^t) \cong \operatorname{Bil}(\mathscr{P} \times \mathscr{P}', \mathscr{F})$. Explicitly we have $\mathscr{P}^t = (P^\vee, Q^t, F^t, F_1^t)$ where $P^\vee = \operatorname{Hom}_S(P, S)$ and

$$Q^t = \{x' \in P^\vee \mid x'(Q) \subseteq I\}.$$

The operators F_1^t and F^t are determined by (2.1) with σ_1 in place of F_1''. If (L, T, Ψ) is a normal representation for $\mathscr{P}$, a normal representation for $\mathscr{P}^t$ is given by $(T^\vee, L^\vee, \Psi^t)$ where $(\Psi^t)^\sharp$ is equal to $((\Psi^\sharp)^{-1})^\vee$. This shows that F_1^t and F^t are well-defined. There is a natural isomorphism $\mathscr{P}^{tt} \cong \mathscr{P}$.
For a more detailed exposition of the duality formalism in the case of (Diedonné) displays we refer to [Z1, Definition 19] or [L2, Section 3].

Lemma 2.14. *Let $\alpha : \mathscr{F} \to \mathscr{F}'$ be a u-homomorphism of frames and let $c \in S'$ be a unit such that $c^{-1}\sigma'(c) = u$. For all $\mathscr{F}$-windows $\mathscr{P}$ there is a natural isomorphism (depending on c)*

$$\alpha_*(\mathscr{P}^t) \cong (\alpha_*\mathscr{P})^t.$$

Proof. We consider the $\mathscr{F}'$-window $\mathscr{F}'_u = (S', I', u\sigma', u\sigma_1')$. The given bilinear form $\mathscr{P} \times \mathscr{P}^t \to \mathscr{F}$ induces a bilinear form $\alpha_*\mathscr{P} \times \alpha_*(\mathscr{P}^t) \to \mathscr{F}'_u$; this is easily verified using that under base change by α each of the operators F_1, F_1', and $F_1'' = \sigma_1$ accounts for one factor of u in (2.1). Multiplication by c is an isomorphism of $\mathscr{F}'$-windows $\mathscr{F}'_u \cong \mathscr{F}'$. The resulting bilinear form $\alpha_*\mathscr{P} \times \alpha_*(\mathscr{P}^t) \to \mathscr{F}'$ induces an isomorphism $\alpha_*(\mathscr{P}^t) \cong (\alpha_*\mathscr{P})^t$. $\square$

3 Crystalline homomorphisms

Definition 3.1. A homomorphism of frames $\alpha : \mathscr{F} \to \mathscr{F}'$ is called crystalline if the functor $\alpha_* : (\mathscr{F}\text{-windows}) \to (\mathscr{F}'\text{-windows})$ is an equivalence of categories.

Theorem 3.2. *Let $\alpha : \mathscr{F} \to \mathscr{F}'$ be a strict frame homomorphism that induces an isomorphism $R \cong R'$ and a surjection $S \to S'$ with kernel $\mathfrak{a} \subset S$. We assume that there is a finite filtration $\mathfrak{a} = \mathfrak{a}_0 \supseteq \cdots \supseteq \mathfrak{a}_n = 0$ with $\sigma(\mathfrak{a}_i) \subseteq \mathfrak{a}_{i+1}$ and $\sigma_1(\mathfrak{a}_i) \subseteq \mathfrak{a}_i$ such that σ_1 is elementwise nilpotent on $\mathfrak{a}_i/\mathfrak{a}_{i+1}$. We assume that finitely generated projective S'-modules lift to projective S-modules. Then α is crystalline.*

In many applications the lifting property of projective modules holds because $\mathfrak{a}$ is nilpotent or S is local. The proof of Theorem 3.2 is a variation of the proofs of [Z1, Theorem 44] and [Z2, Theorem 3].

Proof. The homomorphism α factors into $\mathscr{F} \to \mathscr{F}'' \to \mathscr{F}'$ where the frame $\mathscr{F}''$ is determined by $S'' = S/\mathfrak{a}_1$, so by induction we may assume that $\sigma(\mathfrak{a}) = 0$. The functor α_* is essentially surjective because normal representations (L, T, Ψ) can be lifted from $\mathscr{F}'$ to $\mathscr{F}$. In order that α_* is fully faithful it suffices to show that α_* is fully faithful on automorphisms because a homomorphism $g : \mathscr{P} \to \mathscr{P}'$ can be encoded by the automorphism $\left(\begin{smallmatrix} 1 & 0 \\ g & 1 \end{smallmatrix}\right)$ of $\mathscr{P} \oplus \mathscr{P}'$. Since for a window $\mathscr{P}$ over $\mathscr{F}$ an automorphism of $\alpha_*\mathscr{P}$ can be lifted to an S-module automorphism of P, it suffices to prove the following assertion.

Assume that $\mathscr{P} = (P, Q, F, F_1)$ and $\mathscr{P}' = (P, Q, F', F_1')$ are two $\mathscr{F}$-windows such that $F \equiv F'$ and $F_1 \equiv F_1'$ modulo $\mathfrak{a}$. Then there is a unique $\mathscr{F}$-window isomorphism $g : \mathscr{P} \cong \mathscr{P}'$ with $g \equiv \mathrm{id}$ modulo $\mathfrak{a}$.

We write $F_1' = F_1 + \eta$ and $F' = F + \varepsilon$ and $g = 1 + \omega$, where the σ-linear maps $\eta : Q \to \mathfrak{a}P$ and $\varepsilon : P \to \mathfrak{a}P$ are given, and where $\omega : P \to \mathfrak{a}P$ is an arbitrary S-linear map. The induced g is an isomorphism of windows if and only if $gF_1 = F_1'g$ on Q, which translates into the identity

$$\eta = \omega F_1 - F_1'\omega. \tag{3.1}$$

We fix a normal decomposition $P = L \oplus T$, thus $Q = L \oplus IT$. For $l \in L$, $t \in T$, and $a \in I$ we have

$$\begin{aligned} \eta(l + at) &= \eta(l) + \sigma_1(a)\varepsilon(t), \\ \omega(F_1(l + at)) &= \omega(F_1(l)) + \sigma_1(a)\omega(F(t)), \\ F_1'(\omega(l + at)) &= F_1'(\omega(l)) + \sigma_1(a)F'(\omega(t)). \end{aligned}$$

Here $F'\omega = 0$ because for $a \in \mathfrak{a}$ and $x \in P$ we have $F'(ax) = \sigma(a)F'(x)$, and $\sigma(\mathfrak{a}) = 0$. As $\sigma_1(I)$ generates S we see that (3.1) is equivalent to:

$$\begin{cases} \varepsilon = \omega F & \text{on } T, \\ \eta = \omega F_1 - F_1'\omega & \text{on } L. \end{cases} \tag{3.2}$$

Since $\Psi : L \oplus T \xrightarrow{F_1 + F} P$ is a σ-linear isomorphism, to give ω is equivalent to give a pair of σ-linear maps

$$\omega_L = \omega F_1 : L \to \mathfrak{a}P, \qquad \omega_T = \omega F : T \to \mathfrak{a}P.$$

Let $\lambda : L \to L^{(\sigma)}$ be the composition $L \subseteq P \xrightarrow{(\Psi^\sharp)^{-1}} L^{(\sigma)} \oplus T^{(\sigma)} \xrightarrow{pr_1} L^{(\sigma)}$ and let $\tau : L \to T^{(\sigma)}$ be analogous with pr_2 in place of pr_1. Then the restriction $\omega|_L$ is equal to $\omega_L^\sharp\lambda + \omega_T^\sharp\tau$, and (3.2) becomes:

$$\begin{cases} \omega_T = \varepsilon|_T, \\ \omega_L - F_1'\omega_L^\sharp\lambda = \eta|_L + F_1'\omega_T^\sharp\tau. \end{cases} \tag{3.3}$$

Let $\mathscr{H}$ be the abelian group of σ-linear maps $L \to \mathfrak{a}P$. We claim that the endomorphism U of $\mathscr{H}$ given by $U(\omega_L) = F_1'\omega_L^\sharp\lambda$ is elementwise nilpotent, which implies that $1 - U$ is bijective, and (3.3) has a unique solution in (ω_L, ω_T) and thus in ω. The endomorphism F_1' of $\mathfrak{a}P$ is elementwise nilpotent because $F_1'(ax) = \sigma_1(a)F'(x)$ and because σ_1 is elementwise nilpotent on $\mathfrak{a}$ by assumption. Since L is finitely generated it follows that U is elementwise nilpotent. □

Remark 3.3. The same argument applies if instead of σ_1 being elementwise nilpotent one demands that λ is (topologically) nilpotent, which is the original situation in [Z1, Theorem 44]; see section 10.

4 Abstract deformation theory

Definition 4.1. The Hodge filtration of a window $\mathscr{P}$ is the submodule

$$Q/IP \subseteq P/IP.$$

Lemma 4.2. *Let $\alpha : \mathscr{F} \to \mathscr{F}'$ be a strict homomorphism of frames such that $S = S'$; thus $R \to R'$ is surjective and we have $I \subseteq I'$. Then $\mathscr{F}$-windows $\mathscr{P}$ are equivalent to pairs consisting of an $\mathscr{F}'$-window $\mathscr{P}' = (P', Q', F', F_1')$ and a lift of its Hodge filtration to a direct summand $V \subseteq P'/IP'$.*

Proof. The equivalence is given by the functor $\mathscr{P} \mapsto (\alpha_*\mathscr{P}, Q/IP)$, which is easily seen to be fully faithful. We show that it is essentially surjective. Let an $\mathscr{F}'$-window $\mathscr{P}'$ and a lift of its Hodge filtration $V \subseteq P'/IP'$ be given and let $Q \subseteq P'$ be the inverse image of V; thus $Q \subseteq Q'$. We have to show that $\mathscr{P} = (P', Q, F', F_1'|_Q)$ is an $\mathscr{F}$-window. First we need a normal decomposition for $\mathscr{P}$; this is a decomposition $P' = L \oplus T$ such that $V = L/IL$. Since $\mathscr{P}'$ has a normal decomposition, $\mathscr{P}$ has one too for at least one choice of V. By modifying the isomorphism $P' \cong L \oplus T$ with an automorphism $\left(\begin{smallmatrix} 1 & 0 \\ c & 1 \end{smallmatrix}\right)$ of $L \oplus T$ for some homomorphism $c : L \to I'T$ one reaches every lift of the Hodge filtration. It remains to show that $F_1'(Q)$ generates P'. In terms of a normal decomposition $P' = L \oplus T$ for $\mathscr{P}$ this means that $F_1' + F' : L \oplus T \to P'$ is a σ-linear isomorphism, which holds because $\mathscr{P}'$ is an $\mathscr{F}'$-window. □

Assume that a strict homomorphism of frames $\alpha : \mathscr{F} \to \mathscr{F}'$ is given such that $S \to S'$ is surjective with kernel $\mathfrak{a}$, and $I' = IS'$. We want to factor α into strict frame homomorphisms

$$(S, I, R, \sigma, \sigma_1) \xrightarrow{\alpha_1} (S, I'', R', \sigma, \sigma_1'') \xrightarrow{\alpha_2} (S', I', R', \sigma', \sigma_1') \tag{4.1}$$

such that α_2 satisfies the hypotheses of Theorem 3.2.
Necessarily $I'' = I + \mathfrak{a}$. The main point is to define $\sigma_1'' : I'' \to S$, which is equivalent to defining a σ-linear map $\sigma_1'' : \mathfrak{a} \to \mathfrak{a}$ that extends the restriction of σ_1 to $I \cap \mathfrak{a}$ and satisfies the hypotheses of Theorem 3.2. Once this is achieved, Theorem 3.2 and Lemma 4.2 will show that $\mathscr{F}$-windows are equivalent to $\mathscr{F}'$-windows $\mathscr{P}'$ plus a lift of the Hodge filtration of $\mathscr{P}'$ to a direct summand of P/IP, where $\mathscr{P}'' = (P, Q'', F, F_1'')$ is the unique lift of $\mathscr{P}'$ under α_2.

5 Dieudonné frames

Let R be a noetherian complete local ring with maximal ideal $\mathfrak{m}_R$ and with perfect residue field k of characteristic p. If $p = 2$, we assume that p annihilates R. Let $\hat{W}(\mathfrak{m}_R) \subset W(R)$ be the ideal of all Witt vectors whose coefficients lie in $\mathfrak{m}_R$ and converge to zero $\mathfrak{m}_R$-adically. There is a unique subring $\mathbb{W}(R)$ of $W(R)$ which is stable under the Frobenius f such that the projection $\mathbb{W}(R) \to W(k)$ is surjective with kernel $\hat{W}(\mathfrak{m}_R)$, and the ring $\mathbb{W}(R)$ is also stable under the Verschiebung v; see [Z2, Lemma 2]. Let $\mathbb{I}_R$ be the kernel of the projection to the first component $\mathbb{W}(R) \to R$. Then $v : \mathbb{W}(R) \to \mathbb{I}_R$ is bijective.

Definition 5.1. The Dieudonné frame associated to R is

$$\mathscr{D}_R = (\mathbb{W}(R), \mathbb{I}_R, R, f, f_1)$$

with $f_1 = v^{-1}$.

Here $\theta = p$. Windows over $\mathscr{D}_R$ are Dieudonné displays over R in the sense of [Z2]. We note that $\mathbb{W}(R)$ is a local ring, which guarantees the existence of normal decompositions; see Remark 2.5. The inclusion $\mathbb{W}(R) \to W(R)$ is a strict homomorphism of frames $\mathscr{D}_R \to \mathscr{W}_R$.
If R' has the same properties as R, a local ring homomorphism $R \to R'$ induces a strict frame homomorphism $\mathscr{D}_R \to \mathscr{D}_{R'}$.
Assume that $R' = R/\mathfrak{b}$ for an ideal $\mathfrak{b}$ which is equipped with elementwise nilpotent divided powers γ. Then $\mathbb{W}(R) \to \mathbb{W}(R')$ is surjective with kernel $\hat{W}(\mathfrak{b}) = W(\mathfrak{b}) \cap \hat{W}(\mathfrak{m}_R)$. In this situation, a factorisation (4.1) of the homomorphism $\mathscr{D}_R \to \mathscr{D}_{R'}$ can be defined as follows. We recall that the γ-divided Witt polynomials are defined as

$$w'_n(X_0, \ldots, X_n) = (p^n - 1)!\gamma_{p^n}(X_0) + (p^{n-1} - 1)!\gamma_{p^{n-1}}(X_1) + \cdots + X_n.$$

Thus $p^n w'_n$ is the usual Witt polynomial $w_n(X_0, \ldots, X_n) = X_0^{p^n} + \cdots + p^n X_n$.
Let $\mathfrak{b}^{<\infty>}$ be the $W(R)$-module of all sequences $[b_0, b_1, \ldots]$ with elements $b_i \in \mathfrak{b}$ that converge to zero $\mathfrak{m}_R$-adically, such that $x \in W(R)$ acts on $\mathfrak{b}^{<\infty>}$ by $[b_0, b_1, \ldots] \mapsto [w_0(x)b_0, w_1(x)b_1, \ldots]$. We have an isomorphism of $W(R)$-modules

$$\log : \hat{W}(\mathfrak{b}) \cong \mathfrak{b}^{<\infty>}; \qquad b \mapsto (w'_0(b), w'_1(b), \ldots);$$

see the remark after [Z1, Cor. 82]. For $b \in \hat{W}(\mathfrak{b})$ we call $\log(b)$ the logarithmic coordinates of b. Let

$$\mathbb{I}_{R/R'} = \mathbb{I}_R + \hat{W}(\mathfrak{b}).$$

In logarithmic coordinates, the restriction of f_1 to $\mathbb{I}_R \cap \hat{W}(\mathfrak{b})$ is given by

$$f_1([0, b_1, b_2, \ldots]) = [b_1, b_2, \ldots].$$

Thus $f_1 : \mathbb{I}_R \to \mathbb{W}(R)$ extends uniquely to an f-linear map

$$\tilde{f}_1 : \mathbb{I}_{R/R'} \to \mathbb{W}(R)$$

with $\tilde{f}_1([b_0, b_1, \ldots]) = [b_1, b_2, \ldots]$ on $\hat{W}(\mathfrak{b})$, and we obtain a factorisation

$$\mathscr{D}_R \xrightarrow{\alpha_1} \mathscr{D}_{R/R'} = (\mathbb{W}(R), \mathbb{I}_{R/R'}, R', f, \tilde{f}_1) \xrightarrow{\alpha_2} \mathscr{D}_{R'}. \tag{5.1}$$

Proposition 5.2. *The frame homomorphism α_2 is crystalline.*

This is a reformulation of [Z2, Theorem 3] if $\mathfrak{m}_R$ is nilpotent, and the general case is an easy consequence. As explained in section 4, it follows that deformations of Dieudonné displays from R' to R are classified by lifts of the Hodge filtration; this is [Z2, Theorem 4].

Proof of Proposition 5.2. When $\mathfrak{m}_R$ is nilpotent, α_2 satisfies the hypotheses of Theorem 3.2; the required filtration of $\mathfrak{a} = \hat{W}(\mathfrak{b})$ is $\mathfrak{a}_i = p^i\mathfrak{a}$. In general, these hypotheses are not fulfilled because $f_1 : \mathfrak{a} \to \mathfrak{a}$ is only topologically nilpotent. However, one can find a sequence of ideals $R \supset I_1 \supset I_2 \cdots$ which define the $\mathfrak{m}_R$-adic topology such that each $\mathfrak{b} \cap I_n$ is stable under the divided powers of $\mathfrak{b}$. Indeed, for each n there is an l with $\mathfrak{m}_R^l \cap \mathfrak{b} \subseteq \mathfrak{m}_R^n\mathfrak{b}$; for $I_n = \mathfrak{m}_R^n\mathfrak{b} + \mathfrak{m}_R^l$ we have $\mathfrak{b} \cap I_n = \mathfrak{m}_R^n\mathfrak{b}$. The proposition holds for each R/I_n in place of R, and the general case follows by passing to the projective limit, using Lemma 2.12. □

6 $\varkappa$-frames

The results in this section are essentially due to Th. Zink (private communication); see also [Z3, Section 1] and [VZ1, Section 3].

Definition 6.1. A $\varkappa$-frame is a frame $\mathscr{F} = (S, I, R, \sigma, \sigma_1)$ such that

iv. S has no p-torsion,

v. $W(R)$ has no p-torsion,

vi. $\sigma(\theta) - \theta^p = p \cdot \text{unit in } S$.

The numbering extends i–iii of Definition 2.1. In the following we refer to conditions i–vi without explicitly mentioning Definitions 2.1 and 6.1.

Remark 6.2. If ii and iv hold, we have a (non-additive) map

$$\tau : S \to S, \qquad \tau(x) = \frac{\sigma(x) - x^p}{p},$$

and vi says that $\tau(\theta)$ is a unit. Condition v is satisfied if and only if the nilradical $\mathscr{N}(R)$ has no p-torsion, for example if R is reduced, or flat over $\mathbb{Z}_{(p)}$.

Proposition 6.3. *To each $\varkappa$-frame $\mathscr{F}$ one can associate a u-homomorphism of frames $\varkappa : \mathscr{F} \to \mathscr{W}_R$ lying over id_R for a well-defined unit u of $W(R)$. The homomorphism $\varkappa$ and the unit u are functorial in $\mathscr{F}$ with respect to strict frame homomorphisms.*

Proof. Conditions iv and ii imply that there is a well-defined ring homomorphism $\delta : S \to W(S)$ with $w_n\delta = \sigma^n$; see [Bou, IX.1, proposition 2]. We have $f\delta = \delta\sigma$. Let $\varkappa$ be the composite ring homomorphism

$$\varkappa : S \xrightarrow{\delta} W(S) \to W(R).$$

Then $f\varkappa = \varkappa\sigma$ and $\varkappa(I) \subseteq I_R$. Clearly $\varkappa$ is functorial in $\mathscr{F}$. To define u we write $1 = \sum y_i\sigma_1(x_i)$ in S with $x_i \in I$ and $y_i \in S$. This is possible by iii. Recall that $\theta = \sum y_i\sigma(x_i)$; see the proof of Lemma 2.2. Let

$$u = \sum \varkappa(y_i)f_1\varkappa(x_i).$$

Then $pu = \varkappa(\theta)$ because $pf_1 = f$ and $f\varkappa = \varkappa\sigma$. We claim that $f_1\varkappa = u \cdot \varkappa\sigma_1$. By condition v this is equivalent to the relation $p \cdot f_1\varkappa = pu \cdot \varkappa\sigma_1$, which holds since $pf_1 = f$ and $pu = \varkappa(\theta)$ and $\theta\sigma_1 = \sigma$. It remains to show that u is a unit in $W(R)$. Let $pu = \varkappa(\theta) = (a_0, a_1, \ldots)$ as a Witt vector. By Lemma 6.4 below, u is a unit if and only if a_1 is a unit in R. In $W_2(S)$ we have $\delta(\theta) = (\theta, \tau(\theta))$ because (w_0, w_1) applied to both sides gives $(\theta, \sigma(\theta))$. Hence a_1 is a unit by vi. We conclude that $\varkappa : \mathscr{F} \to \mathscr{W}_R$ is a u-homomorphism of frames.
Finally, u is functorial in $\mathscr{F}$ by its uniqueness, see Remark 2.8. □

Lemma 6.4. *Let R be a ring with $p \in \operatorname{Rad}(R)$ and let $u \in W(R)$ be given. For an integer $r \geq 0$ let $p^r u = (a_0, a_1, a_2, \ldots)$. The element u is a unit in $W(R)$ if and only if a_r is a unit in R.*

Proof. Assume first that $r = 0$. It suffices to show that an element $\bar{u}$ of $W_{n+1}(R)$ that maps to 1 in $W_n(R)$ is a unit. If $\bar{u} = 1 + v^n(x)$ with $x \in R$, then $\bar{u}^{-1} = 1 + v^n(y)$ where $y \in R$ is determined by the equation $x + y + p^n xy = 0$, which has a solution since $p \in \operatorname{Rad}(R)$. For general r, by the case $r = 0$ we may replace R by R/pR. Then we have $p(b_0, b_1, \ldots) = (0, b_0^p, b_1^p, \ldots)$ in $W(R)$, which reduces the assertion to the case $r = 0$. □

Corollary 6.5. *Let $\mathscr{F}$ be a $\varkappa$-frame with $S = W(k)[[x_1, \ldots, x_r]]$ for a perfect field k of odd characteristic p. Assume that σ extends the Frobenius automorphism of $W(k)$ by $\sigma(x_i) = x_i^p$. Then u is a unit in $\mathbb{W}(R)$, and $\varkappa$ induces a u-homomorphism of frames $\varkappa : \mathscr{F} \to \mathscr{D}_R$.*

Proof. We claim that $\delta(S)$ lies in $\mathbb{W}(S)$. Indeed, $\delta(x_i) = [x_i]$ because w_n applied to both sides gives $x_i^{p^n}$. Thus for each multi-exponent $e = (e_1, \ldots, e_r)$ the element $\delta(x^e) = [x^e]$ lies in $\mathbb{W}(S)$. Let $\mathfrak{m}_S$ be the maximal ideal of S. Since $\mathbb{W}(S) = \varprojlim \mathbb{W}(S/\mathfrak{m}_S^n)$ and since for each n all but finitely many x^e lie in $\mathfrak{m}_S^n$, the claim follows. Hence the image of $\varkappa : S \to W(R)$ is contained in $\mathbb{W}(R)$. By its construction the unit u lies in $\mathbb{W}(R)$; it is invertible in $\mathbb{W}(R)$ because the inclusion $\mathbb{W}(R) \to W(R)$ is a local homomorphism of local rings. □

7 The main frame

Let R be a complete regular local ring with perfect residue field k of characteristic $p \geq 3$. We choose a ring homomorphism

$$\mathfrak{S} = W(k)[[x_1, \ldots, x_r]] \xrightarrow{\pi} R$$

such that $x_1, \ldots, x_r$ map to a regular system of parameters of R. Since the graded ring of R is isomorphic to $k[x_1, \ldots, x_r]$, one can find a power series $E_0 \in \mathfrak{S}$ with constant term zero such that $\pi(E_0) = -p$. Let $E = E_0 + p$ and $I = E\mathfrak{S}$. Then $R = \mathfrak{S}/I$. Let $\sigma : \mathfrak{S} \to \mathfrak{S}$ be the ring endomorphism that extends the Frobenius automorphism of $W(k)$ by $\sigma(x_i) = x_i^p$. We have a frame

$$\mathscr{B} = (\mathfrak{S}, I, R, \sigma, \sigma_1)$$

where σ_1 is defined by $\sigma_1(Ey) = \sigma(y)$ for $y \in \mathfrak{S}$.

Lemma 7.1. *The frame $\mathscr{B}$ is a $\varkappa$-frame.*

Proof. Let $\theta \in \mathfrak{S}$ be the element given by Lemma 2.2. The only condition to be checked is that $\tau(\theta)$ is a unit in $\mathfrak{S}$. Let $E_0' = \sigma(E_0)$. Since $\sigma_1(E) = 1$, we have $\theta = \sigma(E) = E_0' + p$. Hence

$$\tau(\theta) = \frac{\sigma(E_0') + p - (E_0' + p)^p}{p} \equiv 1 + \tau(E_0') \mod p.$$

Since the constant term of E_0 is zero, the same is true for $\tau(E_0')$, which implies that $\tau(\theta)$ is a unit as required. □

Thus Proposition 6.3 and Corollary 6.5 give a ring homomorphism $\varkappa$ from $\mathfrak{S}$ to $\mathbb{W}(R)$, which is a u-homomorphism of frames

$$\varkappa : \mathscr{B} \to \mathscr{D}_R.$$

Here the unit $u \in \mathbb{W}(R)$ is determined by the identity $pu = \varkappa\sigma(E)$.

Theorem 7.2. *The frame homomorphism $\varkappa$ is crystalline (Definition 3.1).*

To prove this we consider the following auxiliary frames. Let $J \subset \mathfrak{S}$ be the ideal $J = (x_1, \ldots, x_r)$, and let $\mathfrak{m}_R$ be the maximal ideal of R. For each positive integer a let $\mathfrak{S}_a = \mathfrak{S}/J^a\mathfrak{S}$ and $R_a = R/\mathfrak{m}_R^a$. Then $R_a = \mathfrak{S}_a/E\mathfrak{S}_a$, where E is not a zero divisor in $\mathfrak{S}_a$. There is a well-defined frame

$$\mathscr{B}_a = (\mathfrak{S}_a, I_a, R_a, \sigma_a, \sigma_{1a})$$

such that the projection $\mathfrak{S} \to \mathfrak{S}_a$ is a strict frame homomorphism $\mathscr{B} \to \mathscr{B}_a$. Indeed, σ induces an endomorphism σ_a of $\mathfrak{S}_a$ because $\sigma(J) \subseteq J$, and for $y \in \mathfrak{S}_a$ one can define $\sigma_{1a}(Ey) = \sigma_a(y)$.

For simplicity, the image of u in $\mathbb{W}(R_a)$ is denoted by u as well. The u-homomorphism $\varkappa$ induces a u-homomorphism

$$\varkappa_a : \mathscr{B}_a \to \mathscr{D}_{R_a}$$

because for $e \in \mathbb{N}^r$ we have $\varkappa(x^e) = [x^e]$, which maps to zero in $\mathbb{W}(R_a)$ when $e_1 + \cdots + e_r \geq a$. We note that $\mathscr{B}_a$ is again a $\varkappa$-frame, so the existence of $\varkappa_a$ can also be viewed as a consequence of Proposition 6.3.

Theorem 7.3. *For each positive integer a the homomorphism $\varkappa_a$ is crystalline.*

To prepare for the proof, for each $a \geq 1$ we will construct the following commutative diagram of frames, where vertical arrows are u-homomorphisms and where horizontal arrows are strict.

$$\begin{array}{ccccc} \mathscr{B}_{a+1} & \xrightarrow{\iota} & \tilde{\mathscr{B}}_{a+1} & \xrightarrow{\pi} & \mathscr{B}_a \\ \downarrow{\scriptstyle \varkappa_{a+1}} & & \downarrow{\scriptstyle \tilde{\varkappa}_{a+1}} & & \downarrow{\scriptstyle \varkappa_a} \\ \mathscr{D}_{R_{a+1}} & \xrightarrow{\iota'} & \mathscr{D}_{R_{a+1}/R_a} & \xrightarrow{\pi'} & \mathscr{D}_{R_a} \end{array} \tag{7.1}$$

The upper line is a factorisation (4.1) of the projection $\mathscr{B}_{a+1} \to \mathscr{B}_a$. This means that the frame $\tilde{\mathscr{B}}_{a+1}$ necessarily takes the form

$$\tilde{\mathscr{B}}_{a+1} = (\mathfrak{S}_{a+1}, \tilde{I}_{a+1}, R_a, \sigma_{a+1}, \tilde{\sigma}_{1(a+1)})$$

with $\tilde{I}_{a+1} = E\mathfrak{S}_{a+1} + J^a/J^{a+1}$. We define $\tilde{\sigma}_{1(a+1)} : \tilde{I}_{a+1} \to \mathfrak{S}_{a+1}$ to be the extension of $\sigma_{1(a+1)} : E\mathfrak{S}_{a+1} \to \mathfrak{S}_{a+1}$ by zero on J^a/J^{a+1}. This is well-defined because

$$E\mathfrak{S}_{a+1} \cap J^a/J^{a+1} = E(J^a/J^{a+1})$$

and because for $x \in J^a/J^{a+1}$ we have $\sigma_{1(a+1)}(Ex) = \sigma_{a+1}(x)$, which is zero since $\sigma(J^a) \subseteq J^{ap}$.

The lower line of (7.1) is the factorisation (5.1) with respect to the trivial divided powers on the kernel $\mathfrak{m}_R^a/\mathfrak{m}_R^{a+1}$.

In order that the diagram commutes it is necessary and sufficient that $\tilde{\varkappa}_{a+1}$ is given by the ring homomorphism $\varkappa_{a+1}$.

It remains to show that $\tilde{\varkappa}_{a+1}$ is a u-homomorphism of frames. The only non-trivial condition is that $\tilde{f}_1 \varkappa_{a+1} = u \cdot \varkappa_{a+1}\tilde{\sigma}_{1(a+1)}$ on $\tilde{I}_{a+1}$. This relation holds on $E\mathfrak{S}_{a+1}$ because $\varkappa_{a+1}$ is a u-homomorphism of frames. On J^a/J^{a+1} we have $\varkappa_{a+1}\tilde{\sigma}_{1(a+1)} = 0$ by definition. For $y \in \mathfrak{S}_{a+1}$ and $e \in \mathbb{N}^r$ with $e_1 + \cdots + e_r = a$ we compute

$$\tilde{f}_1(\varkappa_{a+1}(x^e y)) = \tilde{f}_1([x^e]\varkappa_{a+1}(y)) = \tilde{f}_1([x^e])f(\varkappa_{a+1}(y)) = 0$$

because $\log([x^e]) = [x^e, 0, 0, \ldots]$ and thus $\tilde{f}_1([x^e]) = 0$. As these x^e generate J^a, the required relation on $\tilde{I}_{a+1}$ follows. Thus the diagram is constructed.

Proof of Theorem 7.3. We use induction on a. The homomorphism $\varkappa_1$ is crystalline because it is invertible. Assume that $\varkappa_a$ is crystalline for some positive integer a and consider the diagram (7.1). The homomorphism π' is crystalline by Proposition 5.2, while π is crystalline by Theorem 3.2; the required filtration of J^a/J^{a+1} is trivial. Hence $\tilde{\varkappa}_{a+1}$ is crystalline. By Lemma 4.2, lifts of windows under ι or under ι' are classified by lifts of the Hodge filtration. Since $\varkappa_{a+1}$ lies over the identity of R_{a+1} and since $\tilde{\varkappa}_{a+1}$ lies over the identity of R_a, it follows that $\varkappa_{a+1}$ is crystalline too. □

Proof of Theorem 7.2. The frame homomorphism $\varkappa : \mathscr{B} \to \mathscr{D}_R$ is the projective limit of the frame homomorphisms $\varkappa_a : \mathscr{B}_a \to \mathscr{D}_{R_a}$. By Lemma 2.12, $\mathscr{B}$-windows are equivalent to compatible systems of $\mathscr{B}_a$-windows for $a \geq 1$, and $\mathscr{D}_R$-windows are equivalent to compatible systems of $\mathscr{D}_{R_a}$-windows for $a \geq 1$. Thus Theorem 7.2 follows from Theorem 7.3. □

8 Classification of group schemes

The following consequences of Theorem 7.2 are analogous to [VZ1]. Recall that we assume $p \geq 3$. Let $\mathscr{B} = (\mathfrak{S}, I, R, \sigma, \sigma_1)$ be the frame defined in section 7.

Definition 8.1. A Breuil window relative to $\mathfrak{S} \to R$ is a pair (Q, ϕ) where Q is a free $\mathfrak{S}$-module of finite rank and where $\phi : Q \to Q^{(\sigma)}$ is an $\mathfrak{S}$-linear map with cokernel annihilated by E.

Lemma 8.2. *Breuil windows relative to $\mathfrak{S} \to R$ are equivalent to $\mathscr{B}$-windows in the sense of Definition 2.3.*

Proof. This is similar to [VZ1, Lemma 1]. For a $\mathscr{B}$-window (P, Q, F, F_1) the module Q is free over $\mathfrak{S}$ because $I = E\mathfrak{S}$ is free. Hence $F_1^\sharp : Q^{(\sigma)} \to P$ is bijective, and we can define a Breuil window (Q, ϕ) where ϕ is the inclusion $Q \to P$ composed with the inverse of $F_1^\sharp$. Conversely, if (Q, ϕ) is a Breuil window, $\operatorname{Coker}(\phi)$ is a free R-module. Indeed, ϕ is injective because it becomes bijective over $\mathfrak{S}[E^{-1}]$, so $\operatorname{Coker}(\phi)$ has projective dimension at most one over $\mathfrak{S}$, which implies that it is free over R by using depth. Thus one can define a $\mathscr{B}$-window as follows: $P = Q^{(\sigma)}$, the inclusion $Q \to P$ is ϕ, $F_1 : Q \to Q^{(\sigma)}$ is given by $x \mapsto 1 \otimes x$, and $F(x) = F_1(Ex)$. The two constructions are mutually inverse. □

By [Z2], p-divisible groups over R are equivalent to Dieudonné displays over R. Together with Theorem 7.2 and Lemma 8.2 this implies:

Corollary 8.3. *The category of p-divisible groups over R is equivalent to the category of Breuil windows relative to $\mathfrak{S} \to R$.* □

Let us use the following abbreviation: An *admissible torsion $\mathfrak{S}$-module* is a finitely generated $\mathfrak{S}$-module annihilated by a power of p and of projective dimension at most one.

Definition 8.4. A Breuil module relative to $\mathfrak{S} \to R$ is a triple (M, φ, ψ) where M is an admissible torsion $\mathfrak{S}$-module together with $\mathfrak{S}$-linear maps $\varphi : M \to M^{(\sigma)}$ and $\psi : M^{(\sigma)} \to M$ such that $\varphi\psi = E$ and $\psi\varphi = E$.

When R has characteristic zero, each of the maps φ and ψ determines the other one; see Lemma 8.6 below.

Theorem 8.5. *The category of (commutative) finite flat group schemes over R annihilated by a power of p is equivalent to the category of Breuil modules relative to $\mathfrak{S} \to R$.*

This follows from Corollary 8.3 by the arguments of [K1] or [VZ1]. For completeness we give a detailed proof here.

Proof of Theorem 8.5. In this proof, all finite flat group schemes are of p-power order over R, and all Breuil modules or windows are relative to $\mathfrak{S} \to R$.
A homomorphism $g : (Q_0, \phi_0) \to (Q_1, \phi_1)$ of Breuil windows is called an isogeny if it becomes invertible over $\mathfrak{S}[1/p]$. Then g is injective, and its cokernel is naturally a Breuil module; the required ψ is induced by the $\mathfrak{S}$-linear map $E\phi_1^{-1} : Q_1^{(\sigma)} \to Q_1$. A homomorphism $\gamma : G_0 \to G_1$ of p-divisible groups is called an isogeny if it becomes invertible in $\operatorname{Hom}(G_0, G_1) \otimes \mathbb{Q}$. Then γ is a surjection of fppf sheaves, and its kernel is a finite flat group scheme.
We denote isogenies by $X_* = [X_0 \to X_1]$. A homomorphism of isogenies $q : X_* \to Y_*$ is called a quasi-isomorphism if its cone is a short exact sequence. In the case of p-divisible groups this means that q induces an isomorphism of finite flat group schemes on the kernels; in the case of Breuil windows this means that q induces an isomorphism of Breuil modules on the cokernels.
The equivalence between p-divisible groups and Breuil windows preserves isogenies and short exact sequences, and thus also quasi-isomorphisms of isogenies. We note the following two facts.

(a) Each finite flat group scheme over R of p-power order is the kernel of an isogeny of p-divisible groups over R. See [BBM, Théorème 3.1.1].

(b) Each Breuil module is the cokernel of an isogeny of Breuil windows. This is analogous to [VZ1, Proposition 2]; a proof is also given below.

Let us define an additive functor $H \mapsto M(H)$ from finite flat group schemes to Breuil modules. We write each H as the kernel of an isogeny of p-divisible groups $G_0 \to G_1$ and define $M(H)$ as the cokernel of the associated isogeny of Breuil windows. Assume that $h : H \to H'$ is a homomorphism of finite flat group schemes, and H' is written as the kernel of an isogeny of p-divisible groups $G'_0 \to G'_1$. We embed H into $G''_0 = G_0 \oplus G'_0$ by $(1, h)$ and define $G''_1 = G''_0/H$. The coordinate projections $G_0 \leftarrow G''_0 \to G'_0$ induce homomorphisms of isogenies $G_* \leftarrow G''_* \to G'_*$ such that the first map is a quasi-isomorphism, and the composition induces h on the kernels. Let $Q_* \leftarrow Q''_* \to Q'_*$ be the associated homomorphisms of isogenies of Breuil windows. The first map is a quasi-isomorphism, and the composition induces a homomorphism $M(h) : M(H) \to M(H')$ on the cokernels.

One has to show that the construction is independent of the choice and defines an additive functor. This is an easy verification based on the following observation: If a homomorphism of isogenies of p-divisible groups $q : G_* \to G'_*$ induces zero on the kernels, then q is null-homotopic.

The construction of an additive functor $M \mapsto H(M)$ from Breuil modules to finite flat group schemes is analogous. Each M is written as the cokernel of an isogeny of Breuil windows $Q_0 \to Q_1$, and $H(M)$ is defined as the kernel of the associated isogeny of p-divisible groups. If $m : M \to M'$ is a homomorphism of Breuil modules and if M' is written as the cokernel of an isogeny of Breuil windows $Q'_0 \to Q'_1$, let Q''_0 be the kernel of the surjection $Q''_1 = Q_1 \oplus Q'_1 \to M'$ given by $(m, 1)$. The coordinate inclusions $Q_1 \to Q''_1 \leftarrow Q'_1$ induce homomorphisms of isogenies $Q_* \to Q''_* \leftarrow Q'_*$, where the second map is a quasi-isomorphism. The associated homomorphisms of isogenies of p-divisible groups induce a homomorphism of finite flat group schemes $H(m) : H(M) \to H(M')$ on the kernels.

Again, it is easy to verify that this construction is independent of the choice and defines an additive functor, using that a homomorphism of isogenies of Breuil windows is null-homotopic if and only if it induces zero on the cokernels. Clearly the two functors are mutually inverse.

Finally, let us prove (b). If (M, φ, ψ) is a Breuil module, one can find free $\mathfrak{S}$-modules P and Q together with surjective $\mathfrak{S}$-linear maps $\xi : Q \to M$ and $\xi' : P \to M^{(\sigma)}$ and $\mathfrak{S}$-linear maps $\tilde{\varphi} : Q \to P$ and $\tilde{\psi} : P \to Q$ which lift φ and ψ such that $\tilde{\varphi}\tilde{\psi} = E$ and $\tilde{\psi}\tilde{\varphi} = E$. Next one can choose an isomorphism $\alpha : P \cong Q^{(\sigma)}$ compatible with the projections ξ' and $\xi^{(\sigma)}$ to $M^{(\sigma)}$. Let $\phi = \alpha\tilde{\varphi}$. Then (Q, ϕ) is a Breuil window, and (M, φ, ψ) is the cokernel of the isogeny of Breuil windows $(\operatorname{Ker}\xi, \phi') \to (Q, \phi)$, where ϕ' is the restriction of ϕ. ☐

LEMMA 8.6. *If R has characteristic zero, the category of Breuil modules relative to $\mathfrak{S} \to R$ is equivalent to the category of pairs (M, φ) where M is an admissible torsion $\mathfrak{S}$-module and where $\varphi : M \to M^{(\sigma)}$ is an $\mathfrak{S}$-linear map with cokernel annihilated by E.*

Proof. Cf. [VZ1, Proposition 2]. For a non-zero admissible torsion $\mathfrak{S}$-module M the set of zero divisors on M is equal to $\mathfrak{p} = p\mathfrak{S}$ because every associated prime of M has height one and contains p. In particular, $M \to M_{\mathfrak{p}}$ is injective. The hypothesis of the lemma means that $E \notin \mathfrak{p}$. For a given pair (M, φ) as in the lemma this implies that $\varphi_{\mathfrak{p}} : M_{\mathfrak{p}} \to M_{\mathfrak{p}}^{(\sigma)}$ is surjective, thus bijective because both sides have the same finite length. It follows that φ is injective, and (M, φ) is extended uniquely to a Breuil module by $\psi(x) = \varphi^{-1}(Ex)$. ☐

DUALITY

The dual of a Breuil window (Q, ϕ) is the Breuil window $(Q, \phi)^t = (Q^\vee, \psi^\vee)$ where $Q^\vee = \operatorname{Hom}_{\mathfrak{S}}(Q, \mathfrak{S})$ and where $\psi : Q^{(\sigma)} \to Q$ is the unique $\mathfrak{S}$-linear map with $\psi\phi = E$. Here we identify $(Q^{(\sigma)})^\vee$ and $(Q^\vee)^{(\sigma)}$. For a p-divisible group

G over R let $G^\vee$ be the Serre dual of G, and let $\mathbb{M}(G)$ be the Breuil window associated to G by the equivalence of Corollary 8.3.

Proposition 8.7. *There is a functorial isomorphism* $\lambda_G : \mathbb{M}(G^\vee) \cong \mathbb{M}(G)^t$.

Proof. The equivalence between p-divisible groups over R and Dieudonné displays over R is compatible with duality by [L2, Theorem 3.4]. It is easy to see that the equivalence of Lemma 8.2 preserves duality, so it remains to show that the functor $\varkappa_*$ preserves duality as well. By Lemma 2.14 it suffices to find a unit $c \in \mathbb{W}(R)$ with $c^{-1}f(c) = u$. Since E has constant term p, u maps to 1 in $W(k)$ and thus lies in $1 + \hat{W}(\mathfrak{m}_R)$. Hence we can define c^{-1} by the infinite product $uf(u)f^2(u)\cdots$, which converges in $\mathbb{W}(R) = \varprojlim \mathbb{W}(R/\mathfrak{m}^n)$ in the sense that for each n, all but finitely many factors map to 1 in $\mathbb{W}(R/\mathfrak{m}^n)$. □

The dual of a Breuil module $\mathbb{M} = (M, \varphi, \psi)$ is defined as the Breuil module $\mathbb{M}^t = (M^\star, \psi^\star, \varphi^\star)$ where $M^\star = \mathrm{Ext}^1_{\mathfrak{S}}(M, \mathfrak{S})$. Here we identify $(M^{(\sigma)})^\star$ and $(M^\star)^{(\sigma)}$ using that $(\ )^{(\sigma)}$ preserves projective resolutions as σ is flat. For a finite flat group scheme H over R of p-power order let $H^\vee$ be the Cartier dual of H and let $\mathbb{M}(H)$ be the Breuil module associated to H by the equivalence of Theorem 8.5.

Proposition 8.8. *There is a functorial isomorphism* $\lambda_H : \mathbb{M}(H^\vee) \cong \mathbb{M}(H)^t$.

Proof. Choose an isogeny of p-divisible groups $G_0 \to G_1$ with kernel H. Then $\mathbb{M}(H)$ is the cokernel of $\mathbb{M}(G_0) \to \mathbb{M}(G_1)$, which implies that $\mathbb{M}(H)^t$ is the cokernel of $\mathbb{M}(G_1)^t \to \mathbb{M}(G_0)^t$. On the other hand, $H^\vee$ is the kernel of $G_1^\vee \to G_0^\vee$, so $\mathbb{M}(H^\vee)$ is the cokernel of $\mathbb{M}(G_1^\vee) \to \mathbb{M}(G_0^\vee)$. The isomorphisms λ_{G_i} of Proposition 8.7 give an isomorphism $\lambda_H : \mathbb{M}(H^\vee) \cong \mathbb{M}(H)^t$. One easily checks that λ_H is independent of the choice of G_* and functorial in H. □

9 Other lifts of Frobenius

One may ask how much freedom we have in the choice of σ for the frame $\mathscr{B}$. Let $R = \mathfrak{S}/E\mathfrak{S}$ be as in section 7; in particular we assume that $p \geq 3$. Let $J = (x_1, \ldots, x_r)$. To begin with, let $\sigma : \mathfrak{S} \to \mathfrak{S}$ be an arbitrary ring endomorphism such that $\sigma(J) \subset J$ and $\sigma(a) \equiv a^p$ modulo $p\mathfrak{S}$ for $a \in \mathfrak{S}$. We consider the frame

$$\mathscr{B} = (\mathfrak{S}, I, R, \sigma, \sigma_1)$$

with $\sigma_1(Ey) = \sigma(y)$. Again this is a $\varkappa$-frame; the proof of Lemma 7.1 uses only that σ preserves J. Thus Proposition 6.3 gives a homomorphism of frames

$$\varkappa : \mathscr{B} \to \mathscr{W}_R.$$

By the assumptions on σ we have $\sigma(J) \subseteq J^p + pJ$, which implies that the endomorphism $\sigma : J/J^2 \to J/J^2$ is divisible by p.

Proposition 9.1. *The image of* $\varkappa : \mathfrak{S} \to W(R)$ *lies in* $\mathbb{W}(R)$ *if and only if the endomorphism* σ/p *of* J/J^2 *is nilpotent modulo* p.

We have a non-additive map $\tau : J \to J$ given by $\tau(x) = (\sigma(x) - x^p)/p$. Let $\mathfrak{m}$ be the maximal ideal of $\mathfrak{S}$. We write $gr_n(J) = \mathfrak{m}^n J/\mathfrak{m}^{n+1}J$.

Lemma 9.2. *For $n \geq 0$ the map τ preserves $\mathfrak{m}^n J$ and induces a σ-linear endomorphism of k-modules $gr_n(\tau) : gr_n(J) \to gr_n(J)$. We have $gr_0(\tau) = \sigma/p$ as an endomorphism of $gr_0(J) = J/(J^2 + pJ)$. There is a commutative diagram of the following type with $\pi i = \mathrm{id}$*

$$\begin{array}{ccc} gr_n(J) & \xrightarrow{gr_n(\tau)} & gr_n(J) \\ {\scriptstyle\pi}\downarrow & & \uparrow{\scriptstyle i} \\ gr_0(J) & \xrightarrow{gr_0(\tau)} & gr_0(J). \end{array}$$

Proof. Let $J' = p^{-1}\mathfrak{m}J$ as an $\mathfrak{S}$-submodule of $J \otimes \mathbb{Q}$. Then $J \subset J'$, and $gr_n(J)$ is an $\mathfrak{S}$-submodule of $gr_n(J') = \mathfrak{m}^n J'/\mathfrak{m}^{n+1}J'$. The composition $J \xrightarrow{\tau} J \subset J'$ can be written as $\tau = \sigma/p - \varphi/p$, where $\varphi(x) = x^p$. One checks that $\varphi/p : \mathfrak{m}^n J \to \mathfrak{m}^{n+1}J'$ (which requires $p \geq 3$ when $n = 0$) and that $\sigma/p : \mathfrak{m}^n J \to \mathfrak{m}^n J'$. Hence σ/p and τ induce the same map $\mathfrak{m}^n J \to gr_n(J')$. This map is σ-linear and zero on $\mathfrak{m}^{n+1}J$ because this holds for σ/p, and its image lies in $gr_n(J)$ because this is true for τ.
We define $i : gr_0(J) \to gr_n(J)$ by $x \mapsto p^n x$. For $n \geq 1$ let K_n be the image of $\mathfrak{m}^{n-1}J^2 \to gr_n(J)$. Then i maps $gr_0(J)$ bijectively onto $gr_n(J)/K_n$, so there is a unique homomorphism $\pi : gr_n(J) \to gr_0(J)$ with kernel K_n such that $\pi i = \mathrm{id}$. Clearly i commutes with $gr(\tau)$. Thus, in order that the diagram commutes, it suffices that $gr_n(\tau)$ vanishes on K_n. We have $\sigma(J) \subseteq \mathfrak{m}J$, which implies that $(\sigma/p)(\mathfrak{m}^{n-1}J^2) \subseteq \mathfrak{m}^{n+1}J'$, and the assertion follows. □

Proof of Proposition 9.1. Recall that $\varkappa = \pi\delta$, where $\delta : \mathfrak{S} \to W(\mathfrak{S})$ is defined by $w_n\delta = \sigma^n$ for $n \geq 0$, and where $\pi : W(\mathfrak{S}) \to W(R)$ is the obvious projection. For $x \in J$ and $n \geq 1$ let

$$\tau_n(x) = (\sigma(x)^{p^{n-1}} - x^{p^n})/p^n,$$

thus $\tau_1 = \tau$. It is easy to see that

$$\tau_{n+1}(x) \in J \cdot \tau_n(x),$$

in particular we have $\tau_n : J \to J^n$. If $\delta(x) = (y_0, y_1, \ldots)$, the coefficients y_n are determined by $y_0 = x$ and $w_n(y) = \sigma w_{n-1}(y)$ for $n \geq 1$, which translates into the equations

$$y_n = \tau_n(y_0) + \tau_{n-1}(y_1) + \cdots + \tau_1(y_{n-1}).$$

Assume now that σ/p is nilpotent on J/J^2 modulo p. By Lemma 9.2 this implies that $gr_n(\tau)$ is nilpotent for every $n \geq 0$. We will show that for $x \in J$ the element $\delta(x)$ lies is $\mathbb{W}(\mathfrak{S})$, which means that the above sequence (y_n) converges to zero. Assume that for some $N \geq 0$ we have $y_n \in \mathfrak{m}^N J$ for all but finitely

many n. The last two displayed equations give that $y_n - \tau(y_{n-1}) \in \mathfrak{m}^{N+1}J$ for all but finitely many n. As $gr_N(\tau)$ is nilpotent it follows that $y_n \in \mathfrak{m}^{N+1}J$ for all but finitely many n. Thus $\delta(x) \in \mathbb{W}(\mathfrak{S})$ and in particular $\varkappa(x) \in \mathbb{W}(R)$.
Conversely, if σ/p is not nilpotent on J/J^2 modulo p, then $gr_0(\tau)$ is not nilpotent by Lemma 9.2, so there is an $x \in J$ such that $\tau^n(x) \notin \mathfrak{m}J$ for all $n \geq 0$. For $\delta(x) = (y_0, y_1, \ldots)$ we have $y_n \equiv \tau^n x$ modulo $\mathfrak{m}J$. The projection $\mathfrak{S} \to R$ induces an isomorphism $J/\mathfrak{m}J \cong \mathfrak{m}_R/\mathfrak{m}_R^2$. It follows that $\varkappa(x)$ lies in $W(\mathfrak{m}_R)$ but not in $\hat{W}(\mathfrak{m}_R)$, thus $\varkappa(x) \notin \mathbb{W}(R)$. ☐

Now we assume that σ/p is nilpotent on J/J^2 modulo p. Then we have a homomorphism of frames

$$\varkappa : \mathscr{B} \to \mathscr{D}_R.$$

As earlier let $\mathscr{B}_a = (\mathfrak{S}_a, I_a, R_a, \sigma_a, \sigma_{1a})$ with $\mathfrak{S}_a = \mathfrak{S}/J^a$ and $R_a = R/\mathfrak{m}_R^a$. The proof of Lemma 7.1 shows that $\mathscr{B}_a$ is a $\varkappa$-frame. Since $\mathbb{W}(R_a)$ is the image of $\mathbb{W}(R)$ in $W(R_a)$, we get a homomorphism of frames compatible with $\varkappa$:

$$\varkappa_a : \mathscr{B}_a \to \mathscr{D}_{R_a}.$$

Theorem 9.3. *The homomorphisms $\varkappa$ and $\varkappa_a$ are crystalline.*

Proof. The proof is similar to that of Theorems 7.2 and 7.3.
First we repeat the construction of the diagram (7.1). The restriction of $\sigma_{1(a+1)}$ to $E(J^a/J^{a+1}) = p(J^a/J^{a+1})$ is given by $\sigma_1 = \sigma/p = \tau$, which need not be zero in general, but still σ_1 extends uniquely to J^a/J^{a+1} by the formula $\sigma_1 = \sigma/p$. In order that $\tilde{\varkappa}_{a+1}$ is a u-homomorphism of frames we need that $\tilde{f}_1\varkappa_{a+1} = u \cdot \varkappa_{a+1}\tilde{\sigma}_{1(a+1)}$ on J^a/J^{a+1}. Here u acts on J^a/J^{a+1} as the identity. By the proof of Proposition 9.1, for $x \in J^a/J^{a+1}$ we have in $W(J^a/J^{a+1})$

$$\delta(x) = (x, \tau(x), \tau^2(x), \ldots).$$

Since $\tilde{\sigma}_{1(a+1)}(x) = \tau(x)$, the required relation follows easily.
To complete the proof we have to show that $\pi : \tilde{\mathscr{B}}_{a+1} \to \mathscr{B}_a$ is crystalline. Now σ/p is nilpotent modulo p on J^n/J^{n+1} for $n \geq 1$. Indeed, for $n = 1$ this is our assumption, and for $n \geq 2$ the endomorphism σ/p of J^n/J^{n+1} is divisible by p^{n-1} since $\sigma(J) \subseteq pJ + J^p$. In order to apply Theorem 3.2 we need another sequence of auxiliary frames: For $c \in \mathbb{N}$ let $\mathfrak{S}_{a+1,c} = \mathfrak{S}_{a+1}/p^cJ^a\mathfrak{S}_{a+1}$ and let $\tilde{\mathscr{B}}_{a+1,c} = (\mathfrak{S}_{a+1,c}, I_{a+1,c}, R_a, \ldots)$ be the obvious quotient frame of $\tilde{\mathscr{B}}_{a+1}$. Then $\mathscr{B}_a$ is isomorphic to $\tilde{\mathscr{B}}_{a+1,0}$, and $\tilde{\mathscr{B}}_{a+1}$ is the projective limit of $\tilde{\mathscr{B}}_{a+1,c}$ for $c \to \infty$. Theorem 3.2 shows that each projection $\tilde{\mathscr{B}}_{a+1,c+1} \to \tilde{\mathscr{B}}_{a+1,c}$ is crystalline, which implies that π is crystalline by Lemma 2.12. ☐

If σ/p is nilpotent on J/J^2 modulo p, then Corollary 8.3, Theorem 8.5, and the duality Propositions 8.7 and 8.8 follow as before.

10 Nilpotent windows

All results in this article have a nilpotent counterpart where only connected p-divisible groups and nilpotent windows are considered; in this case k need not be perfect and p need not be odd. The necessary modifications are standard, but for completeness we work out the details.

10.1 Nilpotence condition

Let $\mathscr{F} = (S, I, R, \sigma, \sigma_1)$ be a frame. For an $\mathscr{F}$-window $\mathscr{P} = (P, Q, F, F_1)$ there is a unique S-linear map

$$V^\sharp : P \to P^{(\sigma)}$$

with $V^\sharp(F_1(x)) = 1 \otimes x$ for $x \in Q$. In terms of a normal representation $\Psi : L \oplus T \to P$ of $\mathscr{P}$ we have $V^\sharp = (1 \oplus \theta)(\Psi^\sharp)^{-1}$ for θ as in Lemma 2.2. For simplicity, the composition

$$P \xrightarrow{V^\sharp} P^{(\sigma)} \xrightarrow{(V^\sharp)^{(\sigma)}} P^{(\sigma^2)} \to \cdots \to P^{(\sigma^n)}$$

is denoted $(V^\sharp)^n$. The nilpotence condition depends on the choice of an ideal $J \subset S$ such that $\sigma(J) + I + \theta S \subseteq J$, which we call an *ideal of definition* for $\mathscr{F}$.

Definition 10.1. Let $J \subset S$ be an ideal of definition for $\mathscr{F}$. An $\mathscr{F}$-window $\mathscr{P}$ is called nilpotent (with respect to J) if $(V^\sharp)^n \equiv 0$ modulo J for sufficiently large n.

Remark 10.2. For an $\mathscr{F}$-window $\mathscr{P}$ we consider the composition

$$\lambda : L \subseteq L \oplus T \xrightarrow{(\Psi^\sharp)^{-1}} L^{(\sigma)} \oplus T^{(\sigma)} \to L^{(\sigma)}.$$

Then $\mathscr{P}$ is nilpotent if and only if λ is nilpotent modulo J.

10.2 Nil-crystalline homomorphisms

If $\alpha : \mathscr{F} \to \mathscr{F}'$ is a homomorphism of frames and $J \subset S$ and $J' \subset S'$ are ideals of definition with $\alpha(J) \subseteq J'$, the functor α_* preserves nilpotent windows. We call α nil-crystalline if it induces an equivalence between nilpotent $\mathscr{F}$-windows and nilpotent $\mathscr{F}'$-windows. The following variant of Theorem 3.2 formalises [Z1, Theorem 44].

Theorem 10.3. *Let $\alpha : \mathscr{F} \to \mathscr{F}'$ be a homomorphism of frames that induces an isomorphism $R \cong R'$ and a surjection $S \to S'$ with kernel $\mathfrak{a} \subset S$. We assume that there is a finite filtration $\mathfrak{a} = \mathfrak{a}_0 \supseteq \cdots \supseteq \mathfrak{a}_n = 0$ such that $\sigma(\mathfrak{a}_i) \subseteq \mathfrak{a}_{i+1}$ and $\sigma_1(\mathfrak{a}_i) \subseteq \mathfrak{a}_i$. We assume that finitely generated projective S'-modules lift to projective S-modules. If $J \subset S$ is an ideal of definition for $\mathscr{F}$ such that $J^n\mathfrak{a} = 0$ for large n, then α is nil-crystalline with respect to $J \subset S$ and $J' = J/\mathfrak{a} \subset S'$.*

Proof. The assumptions imply that $\mathfrak{a} \subseteq I \subseteq J$, in particular J' is well-defined. An $\mathscr{F}$-window $\mathscr{P}$ is nilpotent if and only if $\alpha_* \mathscr{P}$ is nilpotent. Using this, the proof of Theorem 3.2 applies with the following modification in its final paragraph. We claim that the endomorphism U of $\mathscr{H}$ is nilpotent, which again implies that $1-U$ is bijective. Since $\mathscr{P}$ is nilpotent, λ is nilpotent modulo J, so λ is nilpotent modulo J^n for each $n \geq 1$ as J is stable under σ. Since $J^n \mathfrak{a} = 0$ by assumption, the claim follows from the definition of U. □

10.3 Nilpotent displays

Let R be a ring which is complete and separated in the $\mathfrak{c}$-adic topology for an ideal $\mathfrak{c} \subset R$ containing p. We consider the Witt frame

$$\mathscr{W}_R = (W(R), I_R, R, f, f_1).$$

Here $I_R \subseteq \operatorname{Rad} R$ as required since $W(R) = \varprojlim W_n(R/\mathfrak{c}^n)$ and the successive kernels in this projective system are nilpotent. The inverse image of $\mathfrak{c}$ is an ideal of definition $J \subset W(R)$. Nilpotent windows over $\mathscr{W}_R$ with respect to J are displays over R which are nilpotent over $R/\mathfrak{c}$. By [Z1] and [L1] these are equivalent to p-divisible groups over R which are infinitesimal over $R/\mathfrak{c}$. (Here one uses that displays and p-divisible groups over R are equivalent to compatible systems of the same objects over $R/\mathfrak{c}^n$ for $n \geq 1$; cf. Lemma 2.12 above and [M1, Lemma 4.16].)
Assume that $R' = R/\mathfrak{b}$ for a closed ideal $\mathfrak{b} \subseteq \mathfrak{c}$ equipped with (not necessarily nilpotent) divided powers. One can define a factorisation

$$\mathscr{W}_R \xrightarrow{\alpha_1} \mathscr{W}_{R/R'} = (W(R), I_{R/R'}, R', f, \tilde{f}_1) \xrightarrow{\alpha_2} \mathscr{W}_{R'}$$

of the projection of frames $\mathscr{W}_R \to \mathscr{W}_{R'}$ as follows. Necessarily $I_{R/R'} = I_R + W(\mathfrak{b})$. The divided Witt polynomials define an isomorphism

$$\log : W(\mathfrak{b}) \cong \mathfrak{b}^\infty,$$

and $\tilde{f}_1 : I_{R/R'} \to W(R)$ extends f_1 such that $\tilde{f}_1([b_0, b_1, \ldots]) = [b_1, b_2, \ldots]$ in logarithmic coordinates on $W(\mathfrak{b})$. Let $J' \subset W(R')$ be the image of J. This is an ideal of definition for $\mathscr{W}_{R'}$, and J is an ideal of definition for $\mathscr{W}_{R/R'}$.
We assume that the $\mathfrak{c}$-adic topology of R can be defined by a sequence of ideals $R \supset I_1 \supset I_2 \cdots$ such that $\mathfrak{b} \cap I_n$ is stable under the divided powers of $\mathfrak{b}$ for each n. This is automatic when $\mathfrak{c}$ is nilpotent or when R is noetherian; see the proof of Proposition 5.2.

Proposition 10.4. *The homomorphism α_2 is nil-crystalline with respect to the ideals of definition J for $\mathscr{W}_{R/R'}$ and J' for $\mathscr{W}_{R'}$.*

This is essentially [Z1, Theorem 44].

Proof. By a limit argument the assertion is reduced to the case where $\mathfrak{c} \subset R$ is a nilpotent ideal; see Lemma 2.12. Then Theorem 10.3 applies: The required filtration of $\mathfrak{a} = W(\mathfrak{b})$ is $\mathfrak{a}_i = p^i\mathfrak{a}$. The condition $J^n\mathfrak{a} = 0$ for large n is satisfied because $J^n \subseteq I_R$ for some n and $I_R^{n+1} \subseteq p^nW(R)$ for all n, and $W(\mathfrak{b}) \cong \mathfrak{b}^\infty$ is annihilated by some power of p. □

10.4 The main frame

Let now R be a complete regular local ring with arbitrary residue field k of characteristic p. Let C be a complete discrete valuation ring with maximal ideal pC and residue field k. We choose a surjective ring homomorphism

$$\mathfrak{S} = C[[x_1, \ldots, x_r]] \to R$$

that lifts the identity of k such that $x_1, \ldots, x_r$ map to a regular system of parameters for R. There is a power series $E \in \mathfrak{S}$ with constant term p such that $R = \mathfrak{S}/E\mathfrak{S}$. Let $\sigma : \mathfrak{S} \to \mathfrak{S}$ be a ring endomorphism which induces the Frobenius on $\mathfrak{S}/p\mathfrak{S}$ and preserves the ideal $(x_1, \ldots, x_r)$. Such σ exist because C has a Frobenius lift; see [Gr, Chap. 0, Théorème 19.8.6]. We consider the frame

$$\mathscr{B} = (\mathfrak{S}, I, R, \sigma, \sigma_1)$$

where $\sigma_1(Ey) = \sigma(y)$. Here $\theta = \sigma(E)$. The proof of Lemma 7.1 shows that $\mathscr{B}$ is again a $\varkappa$-frame, so we have a u-homomorphism of frames

$$\varkappa : \mathscr{B} \to \mathscr{W}_R.$$

Let $\mathfrak{m} \subset \mathfrak{S}$ and $\mathfrak{n} \subset W(R)$ be the maximal ideals.

Theorem 10.5. *The homomorphism $\varkappa$ is nil-crystalline with respect to the ideals of definition $\mathfrak{m}$ of $\mathscr{B}$ and $\mathfrak{n}$ of $\mathscr{W}_R$.*

Proof. The proof of Theorem 9.3 applies with the following modification: The initial case $a = 1$ is not trivial because C is not isomorphic to $W(k)$ if k is not perfect, but one can apply [Z3, Theorem 1.6]. In the diagram (7.1) the frame homomorphisms π' and π are only nil-crystalline in general; whether π is crystalline depends on the choice of σ. □

10.5 Connected group schemes

One defines Breuil windows relative to $\mathfrak{S} \to R$ and Breuil modules relative to $\mathfrak{S} \to R$ as before. A Breuil window (Q, ϕ) or a Breuil module (M, φ, ψ) is called nilpotent if ϕ or φ is nilpotent modulo the maximal ideal of $\mathfrak{S}$. The proof of Lemma 8.2 shows that nilpotent Breuil windows are equivalent to nilpotent $\mathscr{B}$-windows. Hence Theorem 10.5 implies:

Corollary 10.6. *Connected p-divisible groups over R are equivalent to nilpotent Breuil windows relative to $\mathfrak{S} \to R$.* □

Similarly we have:

Theorem 10.7. *Connected finite flat group schemes over R of p-power order are equivalent to nilpotent Breuil modules relative to $\mathfrak{S} \to R$.*

This is proved like Theorem 8.5, using two additional remarks:

Lemma 10.8. *Every connected finite flat group scheme H over R is the kernel of an isogeny of connected p-divisible groups.*

Proof. We know that H is the kernel of an isogeny of p-divisible groups $G \to G'$. There is a functorial exact sequence $0 \to G_0 \to G \to G_1 \to 0$ of p-divisible groups where G_0 is connected and G_1 is etale. Since $\operatorname{Hom}(H, G_1)$ is zero, H is the kernel of the isogeny $G_0 \to G_0'$. □

Lemma 10.9. *Every nilpotent Breuil module (M, φ, ψ) relative to $\mathfrak{S} \to R$ is the cokernel of an isogeny of nilpotent Breuil windows.*

Proof. See also [K2, Section 1.3]. As in the proof of Theorem 8.5 we see that (M, φ, ψ) is the cokernel of an isogeny of Breuil windows $(Q, \phi) \to (Q', \phi')$. There is a functorial exact sequence $0 \to Q_0 \to Q \to Q_1 \to 0$ of Breuil windows where Q_0 is nilpotent and where Q_1 is etale in the sense that $\phi : Q_1 \to Q_1^{(\sigma)}$ is bijective. Indeed, by [Z2, Lemma 10] it suffices to construct the sequence over k. Let $\phi_k : Q \otimes_{\mathfrak{S}} k \to Q^{(\sigma)} \otimes_{\mathfrak{S}} k$ be the special fibre of ϕ. Then $Q_0 \otimes_{\mathfrak{S}} k$ is the kernel of the obvious iterate $(\phi_k)^n : Q \otimes_{\mathfrak{S}} k \to Q^{(\sigma^n)} \otimes_{\mathfrak{S}} k$ for large n.
We claim that the free $\mathfrak{S}$-modules Q_1 and Q_1' have the same rank. Let us identify C with $\mathfrak{S}/(x_1, \ldots, x_r)$. Since $Q \to Q'$ becomes bijective over $\mathfrak{S}[1/p]$, the homomorphism $Q \otimes_{\mathfrak{S}} C \to Q' \otimes_{\mathfrak{S}} C$ becomes bijective over $C[1/p]$. Hence the etale parts $(Q \otimes_{\mathfrak{S}} C)_1$ and $(Q' \otimes_{\mathfrak{S}} C)_1$ have the same rank. The claim follows since $(Q \otimes_{\mathfrak{S}} C)_1 = Q_1 \otimes_{\mathfrak{S}} C$ and similarly for Q'.
Let us consider $\bar{M} = Q_1'/Q_1$. Here ϕ' induces a homomorphism $\bar{\varphi} : \bar{M} \to \bar{M}^{(\sigma)}$, which is surjective as Q_1' is etale. The natural surjection $\pi : M \to \bar{M}$ satisfies $\pi^{(\sigma)}\varphi = \bar{\varphi}\pi$. Since φ_k is nilpotent it follows that $\bar{\varphi}_k$ is nilpotent, thus $\bar{M} = 0$ by Nakayama's lemma. Hence $Q_1 \to Q_1'$ is bijective because both sides are free of the same rank, and consequently $M = Q_0'/Q_0$ as desired. □

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Purity Results for p-Divisible Groups and Abelian Schemes over Regular Bases of Mixed Characteristic

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Abstract. Let p be a prime. Let $(R, \mathfrak{m})$ be a regular local ring of mixed characteristic $(0,p)$ and absolute index of ramification e. We provide general criteria of when each abelian scheme over $\operatorname{Spec} R \setminus \{\mathfrak{m}\}$ extends to an abelian scheme over $\operatorname{Spec} R$. We show that such extensions always exist if $e \leq p-1$, exist in most cases if $p \leq e \leq 2p-3$, and do not exist in general if $e \geq 2p-2$. The case $e \leq p-1$ implies the uniqueness of integral canonical models of Shimura varieties over a discrete valuation ring O of mixed characteristic $(0,p)$ and index of ramification at most $p-1$. This leads to large classes of examples of Néron models over O. If $p > 2$ and index $p-1$, the examples are new.

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To Michel Raynaud, for his 71th birthday

1 Introduction

Let p be a prime number. We recall the following *global purity* notion introduced in [V1], Definitions 3.2.1 2) and 9) and studied in [V1] and [V2].

Definition 1 *Let X be a regular scheme that is faithfully flat over* $\operatorname{Spec}\mathbb{Z}_{(p)}$. *We say X is healthy regular (resp. p-healthy regular), if for each open subscheme U of X which contains $X_{\mathbb{Q}}$ and all generic points of $X_{\mathbb{F}_p}$, every abelian scheme (resp. p-divisible group) over U extends uniquely to an abelian scheme (resp. a p-divisible group) over X.*

In (the proofs of) [FC], Chapter IV, Theorems 6.4, 6.4′, and 6.8 was claimed that every regular scheme which is faithfully flat over $\operatorname{Spec}\mathbb{Z}_{(p)}$ is healthy regular as well as p-healthy regular. This claim was disproved by an example of Raynaud–Gabber (see [Ga] and [dJO], Section 6): the regular scheme $\operatorname{Spec} W(k)[[T_1,T_2]]/(p-(T_1T_2)^{p-1})$ is neither p-healthy nor healthy regular. Here $W(k)$ is the ring of Witt vectors with coefficients in a perfect field k of characteristic p. The importance of healthy and p-healthy regular schemes stems from their applications to the study of integral models of *Shimura varieties*. We have a *local* version of Definition 1 as suggested by Grothendieck's work on the classical Nagata–Zariski purity theorem (see [Gr]).

Definition 2 *Let R be a local noetherian ring with maximal ideal $\mathfrak{m}$ such that* $\operatorname{depth} R \geq 2$. *We say that R is quasi-healthy (resp. p-quasi-healthy) if each abelian scheme (resp. p-divisible group) over* $\operatorname{Spec} R\setminus\{\mathfrak{m}\}$ *extends uniquely to an abelian scheme (resp. a p-divisible group) over* $\operatorname{Spec} R$.

If R is local, complete, regular of dimension 2 and mixed characteristic $(0,p)$, then the fact that R is p-quasi-healthy can be restated in terms of finite flat commutative group schemes annihilated by p over $\operatorname{Spec} R$ (cf. Lemma 20).
Our main result is the following theorem proved in Subsections 4.4 and 5.2.

Theorem 3 *Let R be a regular local ring of dimension $d \geq 2$ and of mixed characteristic $(0,p)$. We assume that there exists a faithfully flat local R-algebra $\hat{R}$ which is complete and regular of dimension d, which has an algebraically closed residue class field k, and which is equipped with an epimorphism $\hat{R} \twoheadrightarrow W(k)[[T_1,T_2]]/(p-h)$ where $h \in (T_1,T_2)W(k)[[T_1,T_2]]$ is a power series whose reduction modulo the ideal $(p,T_1^p,T_2^p,T_1^{p-1}T_2^{p-1})$ is non-zero. Then R is quasi-healthy. If moreover $d=2$, then R is also p-quasi-healthy.*

For instance, Theorem 3 applies if the strict completion of R is isomorphic to $W(k)[[T_1,\ldots,T_d]]/(p-T_1\cdot\ldots\cdot T_m)$ with $1\leq m\leq \min\{d,2p-3\}$ (cf. Subsection 5.3). The following consequence is also proved in Subsection 5.2.

Corollary 4 *Let R be a regular local ring of dimension $d \geq 2$ and of mixed characteristic $(0,p)$. Let $\mathfrak{m}$ be the maximal ideal of R. We assume that $p \notin \mathfrak{m}^p$. Then R is quasi-healthy. If moreover $d=2$, then R is also p-quasi-healthy.*

Directly from Theorem 3 and from very definitions we get:

Corollary 5 *Let X be a regular scheme that is faithfully flat over* $\operatorname{Spec}\mathbb{Z}_{(p)}$. *We assume that each local ring R of X of mixed characteristic* $(0,p)$ *and dimension at least 2 is such that the hypotheses of Theorem 3 hold for it (for* *instance, this holds if X is formally smooth over the spectrum of a discrete valuation ring O of mixed characteristic $(0,p)$ and index of ramification $e \leq p-1$). Then X is healthy regular. If moreover $\dim X = 2$, then X is also p-healthy regular.*

The importance of Corollary 5 stems from its applications to *Néron models* (see Section 6). Theorem 31 shows the existence of large classes of new types of Néron models that were not studied before in [N], [BLR], [V1], [V2], or [V3], Proposition 4.4.1. Corollary 5 encompasses (the correct parts of) [V1], Subsubsection 3.2.17 and [V2], Theorem 1.3. Theorem 28 (i) shows that if X is formally smooth over the spectrum of a discrete valuation ring O of mixed characteristic $(0,p)$ and index of ramification e at least p, then in general X is neither p-healthy nor healthy regular. From this and Raynaud–Gabber example we get that Theorem 3 and Corollary 4 are optimal. Even more, if $R = W(k)[[T_1,T_2]]/(p-h)$ with $h \in (T_1,T_2)$, then one would be inclined to expect that R is p-quasi-healthy if and only if h does not belong to the ideal $(p, T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$; this is supported by Theorems 3 and 28 and by Lemma 12. In particular, parts (ii) and (iii) of Theorem 28 present two generalizations of the Raynaud–Gabber example.

Our proofs are based on the classification of finite flat commutative group schemes of p power order over the spectrum of a local, complete, regular ring R of mixed characteristic $(0,p)$ and perfect residue class field. For $\dim R = 1$ this classification was a conjecture of Breuil [Br] proved by Kisin in [K1] and [K2] and reproved by us in [VZ], Theorem 1. Some cases with $\dim R \geq 2$ were also treated in [VZ]. The general case is proved by Lau in [L1], Theorems 1.2 and 10.7. Proposition 15 provides a new proof of Raynaud's result [R2], Corollary 3.3.6.

Subsection 5.1 disproves an additional claim of [FC], Chapter V, Section 6. It is the claim of [FC], top of p. 184 on torsors of liftings of p-divisible groups which was not previously disproved and which unfortunately was used in [V1] and [V2], Subsection 4.3. This explains why our results on p-healthy regular schemes and p-quasi-healthy regular local rings work only for dimension 2 (the difficulty is for the passage from dimension 2 to dimension 3). Implicitly, the p-healthy part of [V2], Theorem 1.3 is proved correctly in [V2] only for dimension 2.

The paper is structured as follows. Different preliminaries on *Breuil windows* and *modules* are introduced in Section 2. In Section 3 we study morphisms between Breuil modules. Our basic results on extending properties of finite flat group schemes, p-divisible groups, and abelian schemes are presented in Sections 4 and 5. Section 6 contains applications to integral models and Néron models.

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2 Preliminaries

In this paper the notions of *frame* and *window* are in a more general sense than in [Z1]. The new notions are suggested by the works [Br], [K1], [VZ], and [L1]. In all that follows we assume that a ring is unitary and commutative and that a finite flat group scheme is commutative and (locally) of p power order.

Definition 6 *A frame $\mathcal{F} = (R, S, J, \sigma, \dot{\sigma}, \theta)$ for a ring R consists of the following data:*

- *(a) A ring S and an ideal $J \subset S$.*
- *(b) An isomorphism of rings $S/J \cong R$.*
- *(c) A ring homomorphism $\sigma : S \to S$.*
- *(d) A σ-linear map $\dot{\sigma} : J \to S$.*
- *(e) An element $\theta \in S$.*

We assume that $pS + J$ is in the radical of S, that σ induces the Frobenius endomorphism on S/pS, and that the following equation holds:

$$\sigma(\eta) = \theta\dot{\sigma}(\eta), \quad \textit{for all } \eta \in J. \tag{1}$$

Assume that

$$S\dot{\sigma}(J) = S. \tag{2}$$

In this case we find an equation $1 = \sum_i \xi_i \dot{\sigma}(\eta_i)$ with $\xi_i \in S$ and $\eta_i \in J$. From this and (1) we get that $\theta = \sum_i \xi_i \sigma(\eta_i)$. Therefore for each $\eta \in J$ we have

$$\sigma(\eta) = \sum_i \xi_i \sigma(\eta)\dot{\sigma}(\eta_i) = \sum_i \xi_i \dot{\sigma}(\eta\eta_i) = \sum_i \xi_i \sigma(\eta_i)\dot{\sigma}(\eta) = \theta\dot{\sigma}(\eta).$$

We conclude that the equation (2) implies the existence and uniqueness of an element θ such that the equation (1) is satisfied.
If M is an S-module we set $M^{(\sigma)} := S \otimes_{\sigma,S} M$. The linearization of a σ-linear map $\phi : M \to N$ is denoted by $\phi^\sharp : M^{(\sigma)} \to N$.

Definition 7 *A window with respect to $\mathcal{F}$ is a quadruple $(P, Q, F, \dot{F})$ where:*

- *(a) P is a finitely generated projective S-module.*
- *(b) $Q \subset P$ is an S-submodule.*
- *(c) $F : P \to P$ is a σ-linear map.*

(d) $\dot{F}: Q \to P$ *is a* σ*-linear map.*

We assume that the following three conditions are satisfied:

(i) *There exists a decomposition* $P = T \oplus L$ *such that* $Q = JT \oplus L$.

(ii) $F(y) = \theta \dot{F}(y)$ *for* $y \in Q$ *and* $\dot{F}(\eta x) = \dot{\sigma}(\eta)F(x)$ *for* $x \in P$ *and* $\eta \in J$.

(iii) $F(P)$ *and* $\dot{F}(Q)$ *generate* P *as an* S*-module.*

If (2) holds, then from the second part of (ii) we get that for $x \in P$ we have $F(x) = 1F(x) = \sum_i \xi_i \dot{\sigma}(\eta_i)F(x) = \sum_i \xi_i \dot{F}(\eta_i x)$; if moreover $x \in Q$, then $F(x) = \sum_i \xi_i \sigma(\eta_i)\dot{F}(x) = \theta \dot{F}(x)$. Thus if (2) holds, then we have an inclusion $F(P) \subset S\dot{F}(Q)$ and the first condition of (ii) follows from the second condition of (ii). A decomposition as in (i) is called a *normal decomposition*.
We note that for each window $(P, Q, F, \dot{F})$ as above, the S-linear map

$$F^\sharp \oplus \dot{F}^\sharp : S \otimes_{\sigma,S} T \oplus S \otimes_{\sigma,S} L \to T \oplus L \tag{3}$$

is an isomorphism. Conversely an arbitrary isomorphism (3) defines uniquely a window with respect to $\mathcal{F}$ equipped with a given normal decomposition.
Let R be a regular local ring of mixed characteristic $(0, p)$. Let $\mathfrak{m}$ be the maximal ideal of R and let $k := R/\mathfrak{m}$.
A finite flat group scheme H over $\operatorname{Spec} R$ is called *residually connected* if its special fibre H_k over $\operatorname{Spec} k$ is connected (i.e., has a trivial étale part). If R is complete, then H is residually connected if and only if H as a scheme is connected and therefore in this case we will drop the word residually. We apply the same terminology to p-divisible groups over $\operatorname{Spec} R$.
In this section we will assume moreover that k is perfect and that R is complete (in the $\mathfrak{m}$-adic topology). Let $d = \dim R \geq 1$.
We choose regular parameters $t_1, \ldots, t_d$ of R. We denote by $W(\dagger)$ the ring of Witt vectors with coefficients in a ring $\dagger$. We set $\mathfrak{S} := W(k)[[T_1, \ldots, T_d]]$. We consider the epimorphism of rings

$$\mathfrak{S} \twoheadrightarrow R,$$

which maps each indeterminate T_i to t_i.
Let $h \in \mathfrak{S}$ be a power series without constant term such that we have

$$p = h(t_1, \ldots, t_d).$$

We set $E := p - h \in \mathfrak{S}$. Then we have a canonical isomorphism

$$\mathfrak{S}/E\mathfrak{S} \cong R.$$

As R is a regular local ring of mixed characteristic $(0, p)$, we have $E \notin p\mathfrak{S}$. We extend the Frobenius automorphism σ of $W(k)$ to $\mathfrak{S}$ by the rule

$$\sigma(T_i) = T_i^p.$$

Note that $\sigma : \mathfrak{S} \to \mathfrak{S}$ is flat. Let $\dot{\sigma} : E\mathfrak{S} \to \mathfrak{S}$ be the σ-linear map defined by the rule

$$\dot{\sigma}(Es) := \sigma(s).$$

Definition 8 *We refer to the sextuple* $\mathcal{L} = (R, \mathfrak{S}, E\mathfrak{S}, \sigma, \dot{\sigma}, \sigma(E))$ *as a standard frame for the ring* R. *A window for this frame will be called a Breuil window.*

As $\dot{\sigma}(E) = 1$, the condition (2) holds for $\mathcal{L}$. Let $\hat{W}(R) \subset W(R)$ be the subring defined in [Z2], Introduction and let σ_R be its Frobenius endomorphism. There exists a natural ring homomorphism

$$\varkappa : \mathfrak{S} \to \hat{W}(R)$$

which commutes with the Frobenius endomorphisms, i.e. for all $s \in \mathfrak{S}$ we have

$$\varkappa(\sigma(s)) = \sigma_R(\varkappa(s)).$$

The element $\varkappa(T_i)$ is the Teichmüller representative $[t_i] \in \hat{W}(R)$ of t_i.

Theorem 9 *(Lau [L1], Theorem 1.1) If* $p \geq 3$, *then the category of Breuil windows is equivalent to the category of* p*-divisible groups over* $\operatorname{Spec} R$.

This theorem was proved first in some cases in [VZ], Theorem 1. As in [VZ], the proof in [L1] shows first that the category of Breuil windows is equivalent (via $\varkappa$) to the category of Dieudonné displays over $\hat{W}(R)$. Theorem 9 follows from this and the fact (see [Z2], Theorem) that the category of Dieudonné displays over $\hat{W}(R)$ is equivalent to the category of p-divisible groups over $\operatorname{Spec} R$.
There exists a version of Theorem 9 for connected p-divisible groups over $\operatorname{Spec} R$ as described in the introductions of [VZ] and [L1]. This version holds as well for $p = 2$, cf. [L1], Corollary 10.6.
The categories of Theorem 9 have natural exact structures [Me2]. The equivalence of Theorem 9 (or of its version for $p \geq 2$) respects the exact structures.
For a prime ideal $\mathfrak{p}$ of R which contains p, let $\kappa(\mathfrak{p})^{\mathrm{perf}}$ be the perfect hull of the residue class field $\kappa(\mathfrak{p})$ of $\mathfrak{p}$. We deduce from $\varkappa$ a ring homomorphism $\varkappa_{\mathfrak{p}} : \mathfrak{S} \to W(\kappa(\mathfrak{p})^{\mathrm{perf}}) = \hat{W}(\kappa(\mathfrak{p})^{\mathrm{perf}})$.

Proposition 10 *Let* G *be a* p*-divisible group over* R. *If* $p = 2$, *we assume that* G *is connected. Let* $(P, Q, F, \dot{F})$ *be the Breuil window of* G. *Then the classical Dieudonné module of* $G_{\kappa(\mathfrak{p})^{\mathrm{perf}}}$ *is canonically isomorphic (in a functorial way) to* $W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}}, \mathfrak{S}} P$ *endowed with the* $\sigma_{\kappa(\mathfrak{p})^{\mathrm{perf}}}$*-linear map* $\sigma_{\kappa(\mathfrak{p})^{\mathrm{perf}}} \otimes F$.

Proof. If G is connected, we consider its display $(P', Q', F', \dot{F}')$ over $W(R)$. By [L1], Theorem 1.1 and Corollary 10.6 we have $P' = W(R) \otimes_{\varkappa, \mathfrak{S}} P$. Let us denote by $\mathbb{D}(G)$ the Grothendieck–Messing crystal associated to G, cf. [Me1]. By [Z1], Theorem 6 there is a canonical and functorial isomorphism $\mathbb{D}(G)_{W(R)} \cong P' \cong W(R) \otimes_{\varkappa, \mathfrak{S}} P$. The functor $\mathbb{D}$ commutes with base change. If we apply this

to the morphism of pd-extensions $W(R) \to W(\kappa(\mathfrak{p})^{\mathrm{perf}})$ of R and $\kappa(\mathfrak{p})^{\mathrm{perf}}$ (respectively), we get that $\mathbb{D}(G_{\kappa(\mathfrak{p})^{\mathrm{perf}}}) \cong \mathbb{D}(G)_{W(\kappa(\mathfrak{p})^{\mathrm{perf}})} \cong W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}},\mathfrak{S}} P$. From this the proposition follows provided G is connected.
In the case $p \geq 3$ the same argument works if we replace $(P', Q', F', \dot{F}')$ by the Dieudonné display of G over $\hat{W}(R)$. But in this case the isomorphism $\mathbb{D}(G)_{\hat{W}(R)} \cong P'$ follows from [L2], Theorem 6.9. □

All results in this paper are actually independent of the nonconnected part of the last Proposition. This is explained in the proof of Corollary 21.
In what follows we will not need to keep track of the $\sigma_{\kappa(\mathfrak{p})^{\mathrm{perf}}}$-linear maps $\sigma_{\kappa(\mathfrak{p})^{\mathrm{perf}}} \otimes F$ and thus we will simply call $W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}},\mathfrak{S}} P$ the fibre of the Breuil window $(P, Q, F, \dot{F})$ over $\mathfrak{p}$.
We often write a Breuil window in the form (Q, ϕ) originally proposed by Breuil, where ϕ is the composite of the inclusion $Q \subset P$ with the inverse of the $\mathfrak{S}$-linear isomorphism $\dot{F}^{\sharp} : Q^{(\sigma)} \cong P$. In this notation P, F, and $\dot{F}$ are omitted as they are determined naturally by $\dot{F}^{\sharp}$ and thus by ϕ (see [VZ], Section 2). A Breuil window in this form is characterized as follows: Q is a finitely generated free $\mathfrak{S}$-module and $\phi : Q \to Q^{(\sigma)}$ is a $\mathfrak{S}$-linear map whose cokernel is annihilated by E. We note that this implies easily that there exists a unique $\mathfrak{S}$-linear map $\psi : Q^{(\sigma)} \to Q$ such that we have

$$\phi \circ \psi = E \,\mathrm{id}_{Q^{(\sigma)}}, \quad \psi \circ \phi = E \,\mathrm{id}_Q .$$

Clearly the datum (Q, ψ) is equivalent to the datum (Q, ϕ). In the notation (Q, ϕ), its fibre over $\mathfrak{p}$ is $W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}},\mathfrak{S}} Q^{(\sigma)} = W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}},\mathfrak{S}} Q$.
The dual of a Breuil window is defined as follows. Let M be a $\mathfrak{S}$-module. We set $\hat{M} := \mathrm{Hom}_{\mathfrak{S}}(M, \mathfrak{S})$. A $\mathfrak{S}$-linear map $M \to \mathfrak{S}$ defines a homomorphism $M^{(\sigma)} \to \mathfrak{S}^{(\sigma)} = \mathfrak{S}$. This defines a $\mathfrak{S}$–linear map:

$$\hat{M}^{(\sigma)} = \mathfrak{S} \otimes_{\sigma,\mathfrak{S}} \mathrm{Hom}_{\mathfrak{S}}(M, \mathfrak{S}) \to \mathrm{Hom}_{\mathfrak{S}}(M^{(\sigma)}, \mathfrak{S}) = \widehat{M^{(\sigma)}}.$$

It is clearly an isomorphism if M is a free $\mathfrak{S}$-module of finite rank and therefore also if M is a finitely generated $\mathfrak{S}$-module by a formal argument which uses the flatness of $\sigma : \mathfrak{S} \to \mathfrak{S}$.
If (Q, ϕ) is a Breuil window we obtain a $\mathfrak{S}$-linear map

$$\hat{\phi} : \hat{Q}^{(\sigma)} = \widehat{(Q^{(\sigma)})} \to \hat{Q}.$$

More symmetrically we can say that if (Q, ϕ, ψ) is a Breuil window then $(\hat{Q}, \hat{\psi}, \hat{\phi})$ is a Breuil window. We call $(\hat{Q}, \hat{\psi}, \hat{\phi})$ the *dual Breuil window* of (Q, ϕ, ψ).
Taking the fibre of a Breuil window (Q, ϕ) over $\mathfrak{p}$ is compatible with duals as we have:

$$W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}},\mathfrak{S}} \hat{Q}^{(\sigma)} \cong \mathrm{Hom}_{W(\kappa(\mathfrak{p})^{\mathrm{perf}})}(W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}},\mathfrak{S}} Q^{(\sigma)}, W(\kappa(\mathfrak{p})^{\mathrm{perf}})). \tag{4}$$

We recall from [VZ], Definition 2 and [L1] that a *Breuil module* (M, φ) is a pair, where M is a finitely generated $\mathfrak{S}$-module which is of projective dimension at most 1 and which is annihilated by a power of p and where $\varphi : M \to M^{(\sigma)}$ is a $\mathfrak{S}$-linear map whose cokernel is annihilated by E. We note that the map φ is always injective (the argument for this is the same as in [VZ], Proposition 2 (i)). It follows formally that there exists a unique $\mathfrak{S}$-linear map $\vartheta : M^{(\sigma)} \to M$ such that we have

$$\varphi \circ \vartheta = E \,\mathrm{id}_{M^{(\sigma)}}, \quad \vartheta \circ \varphi = E \,\mathrm{id}_M .$$

We define the *dual Breuil module* $(M^*, \vartheta^*, \varphi^*)$ of (M, φ, ϑ) by applying the functor $M^* = \mathrm{Ext}^1_{\mathfrak{S}}(M, \mathfrak{S})$ in the same manner we did for windows. It is easy to see that the $\mathfrak{S}$-module M^* has projective dimension at most 1. The fibre of (M, φ) (or of (M, φ, ϑ)) over $\mathfrak{p}$ is

$$W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\varkappa_{\mathfrak{p}}, \mathfrak{S}} M^{(\sigma)} = W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}}, \mathfrak{S}} M. \tag{5}$$

The duals are again compatible with taking fibres as we have:

$$\begin{aligned} &W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}}, \mathfrak{S}} M^* \cong \\ &\quad\cong \mathrm{Ext}^1_{W(\kappa(\mathfrak{p})^{\mathrm{perf}})}(W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}}, \mathfrak{S}} M, W(\kappa(\mathfrak{p})^{\mathrm{perf}})) \\ &\quad= \mathrm{Hom}_{W(\kappa(\mathfrak{p})^{\mathrm{perf}})}(W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}}, \mathfrak{S}} M, W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\mathbb{Z}} \mathbb{Q}). \end{aligned} \tag{6}$$

Assume that p annihilates M, i.e. M is a module over $\bar{\mathfrak{S}} = \mathfrak{S}/p\mathfrak{S}$. As depth M is the same over either $\mathfrak{S}$ or $\bar{\mathfrak{S}}$ and it is d if $M \neq 0$, we easily get that M is a free $\bar{\mathfrak{S}}$-module. From this we get that $M^* = \mathrm{Hom}_{\bar{\mathfrak{S}}}(M, \bar{\mathfrak{S}})$ (to be compared with the last isomorphism of (6)). Thus in this case the duality works exactly as for windows.

If $p \geq 3$, it follows from Theorem 9 that the category of finite flat group schemes over $\mathrm{Spec}\, R$ is equivalent to the category of Breuil modules (the argument for this is the same as for [VZ], Theorem 2). We have a variant of this for $p = 2$ (cf. [L1], Theorem 10.7): the category of connected finite flat group schemes over $\mathrm{Spec}\, R$ is equivalent to the category of nilpotent Breuil modules (i.e., of Breuil modules (M, φ) that have the property that the reduction of φ modulo the maximal ideal of $\mathfrak{S}$ is nilpotent in the natural way).

We recall from [VZ], Subsection 6.1 that the Breuil module of a finite flat group scheme H over $\mathrm{Spec}\, R$ is obtained as follows. By a theorem of Raynaud (see [BBM], Theorem 3.1.1) we can represent H as the kernel

$$0 \to H \to G_1 \to G_2 \to 0$$

of an isogeny $G_1 \to G_2$ of p-divisible groups over $\mathrm{Spec}\, R$. If $p = 2$, then we assume that H and G_1 are connected. Let (Q_1, ϕ_1) and (Q_2, ϕ_2) be the Breuil windows of G_1 and G_2 (respectively). Then the Breuil module (M, φ) of H is the cokernel of the induced map $(Q_1, \phi_1) \to (Q_2, \phi_2)$ in a natural sense. From Proposition 10 we get that the classical covariant Dieudonné module of $H_{\kappa(\mathfrak{p})^{\mathrm{perf}}}$ is canonically given by (5).

3 Morphisms between Breuil modules

In this section, let R be a complete regular local ring of mixed characteristic $(0,p)$ with maximal ideal $\mathfrak{m}$ and perfect residue class field k. We write $R = \mathfrak{S}/E\mathfrak{S}$, where $d = \dim R \geq 1$, $\mathfrak{S} = W(k)[[T_1,\ldots,T_d]]$, and $E = p - h \in \mathfrak{S}$ are as in Section 2. We use the standard frame $\mathcal{L}$ of the Definition 8.
Let $e \in \mathbb{N}^*$ be such that $p \in \mathfrak{m}^e \setminus \mathfrak{m}^{e+1}$. It is the absolute ramification index of R. Let $\bar{\mathfrak{t}} := (T_1,\ldots,T_d) \subset \bar{\mathfrak{S}} := \mathfrak{S}/p\mathfrak{S} = k[[T_1,\ldots,T_d]]$. Let $\bar{h} \in \bar{\mathfrak{t}} \subset \bar{\mathfrak{S}}$ be the reduction modulo p of h. The surjective function $\mathrm{ord} : \bar{\mathfrak{S}} \twoheadrightarrow \mathbb{N} \cup \{\infty\}$ is such that $\mathrm{ord}(\bar{\mathfrak{t}}^i \setminus \bar{\mathfrak{t}}^{i+1}) = i$ for all $i \geq 0$ and $\mathrm{ord}(0) = \infty$.
Let $\mathrm{gr}\, R := \mathrm{gr}_{\mathfrak{m}}\, R$. The obvious isomorphism of graded rings

$$k[T_1,\ldots,T_d] \to \mathrm{gr}\, R \tag{7}$$

maps the initial form of $\bar{h}$ to the initial form of p. Thus e is the order of the power series $\bar{h}$.

Lemma 11 *We assume that R is such that $p \notin \mathfrak{m}^p$ (i.e., $e \leq p-1$). Let C be a $\mathfrak{S}$-module which is annihilated by a power of p. Let $\varphi : C \to C^{(\sigma)}$ be a $\mathfrak{S}$-linear map whose cokernel is annihilated by E. We assume that there exists a power series $f \in \mathfrak{S} \setminus p\mathfrak{S}$ which annihilates C. Then we have:*

(a) If $p \notin \mathfrak{m}^{p-1}$ (i.e., if $e \leq p-2$), then $C = 0$.

(b) If $e = p-1$, then either $C = 0$ or the initial form of p in $\mathrm{gr}\, R$ generates an ideal which is a $(p-1)$-th power.

Proof. It suffices to show that $C = 0$ provided either $e \leq p-2$ or $e = p-1$ and the initial form of p in $\mathrm{gr}\, R$ generates an ideal which is not a $(p-1)$-th power. By the lemma of Nakayama it suffices to show that $C/pC = 0$. It is clear that φ induces a $\mathfrak{S}$-linear map $C/pC \to (C/pC)^{(\sigma)}$. Therefore we can assume that C is annihilated by p.
Let u be the smallest non-negative integer with the following property: for each $c \in C$ there exists a power series $g_c \in \bar{\mathfrak{S}}$ such that $\mathrm{ord}(g_c) \leq u$ and g_c annihilates c.
From the existence of f in the annihilator of C we deduce that the number u exists. If $C \neq 0$, then we have $u > 0$. We will show that the assumption that $u > 0$ leads to a contradiction and therefore we have $C = 0$.
By the minimality of u there exists an element $x \in C$ such that for each power series a in the annihilator $\mathfrak{a} \subset \bar{\mathfrak{S}}$ of x we have $\mathrm{ord}(a) \geq u$. Consider the $\bar{\mathfrak{S}}$-linear injection

$$\bar{\mathfrak{S}}/\mathfrak{a} \hookrightarrow C \tag{8}$$

which maps 1 to x. Let $\mathfrak{a}^{(p)} \subset \bar{\mathfrak{S}}$ be the ideal generated by the p-th powers of elements in $\mathfrak{a}$. Each power series in $\mathfrak{a}^{(p)}$ has order $\geq pu$.
If we tensorize the injection (8) by $\sigma : \bar{\mathfrak{S}} \to \bar{\mathfrak{S}}$ we obtain a $\bar{\mathfrak{S}}$-linear injection

$$\bar{\mathfrak{S}}/\mathfrak{a}^{(p)} \cong \bar{\mathfrak{S}} \otimes_{\sigma,\bar{\mathfrak{S}}} \bar{\mathfrak{S}}/\mathfrak{a} \hookrightarrow C^{(\sigma)}.$$

Thus each power series in the annihilator of $1 \otimes x \in C^{(\sigma)}$ has at least order pu. On the other hand the cokernel of φ is by assumption annihilated by $\bar{h}$. Thus $\bar{h}(1 \otimes x)$ is in the image of φ. By the definition of u we find a power series $g \in \bar{\mathfrak{S}}$ with $\mathrm{ord}(g) \leq u$ which annihilates $\bar{h}(1 \otimes x)$. Thus $g\bar{h} \in \mathfrak{a}^{(p)}$. We get

$$u + \mathrm{ord}(\bar{h}) \geq \mathrm{ord}(g\bar{h}) \geq pu.$$

Therefore $e = \mathrm{ord}(\bar{h}) \geq (p-1)u \geq p-1$. In the case (a) we obtain a contradiction which shows that $C = 0$.
In the case $e = p-1$ we obtain a contradiction if $u > 1$. Assume that $u = 1$. As $g\bar{h} \in \mathfrak{a}^{(p)}$ and as $\mathrm{ord}(g\bar{h}) = p$, there exists a power series $\bar{f} \in \bar{\mathfrak{S}}$ of order 1 and a non-zero element $\xi \in k$ such that

$$g\bar{h} \equiv \xi \bar{f}^p \bmod \bar{\mathfrak{r}}^{p+1}.$$

This shows that the initial forms of g and $\bar{f}$ in the graded ring $\mathrm{gr}_{\bar{\mathfrak{r}}}\,\bar{\mathfrak{S}}$ differ by a constant in k. If we divide the last congruence by $\bar{f}$ we obtain

$$\bar{h} \equiv \xi \bar{f}^{p-1} \bmod \bar{\mathfrak{r}}^p.$$

By the isomorphism (7) this implies that initial form of p in $\mathrm{gr}\, R$ generates an ideal which is a $(p-1)$-th power. Contradiction. □

Lemma 12 *We assume that $d = 2$ and we consider the ring $\bar{\mathfrak{S}} = k[[T_1, T_2]]$. Let $\bar{h} \in \bar{\mathfrak{S}}$ be a power series of order $e \in \mathbb{N}^*$. Then the following two statements are equivalent:*

- *(a) The power series $\bar{h}$ does not belong to the ideal $\bar{\mathfrak{r}}^{(p)} + \bar{\mathfrak{r}}^{2(p-1)} = (T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$ of $\bar{\mathfrak{S}}$.*
- *(b) If C is a $\bar{\mathfrak{S}}$-module of finite length equipped with a $\bar{\mathfrak{S}}$-linear map $\varphi : C \to C^{(\sigma)}$ whose cokernel is annihilated by $\bar{h}$, then C is zero.*

Proof. We consider the $\bar{\mathfrak{S}}$-linear map

$$\tau : k = k[[T_1, T_2]]/(T_1, T_2) \to k^{(\sigma)} = k[[T_1, T_2]]/(T_1^p, T_2^p)$$

that maps 1 to $T_1^{p-1}T_2^{p-1}$ modulo (T_1^p, T_2^p). If $\bar{h} \in \bar{\mathfrak{r}}^{(p)} + \bar{\mathfrak{r}}^{2(p-1)}$, then the cokernel of τ is annihilated by $\bar{h}$. From this we get that (b) implies (a).
Before proving the other implication, we first make some general remarks. The Frobenius endomorphism $\sigma : \bar{\mathfrak{S}} \to \bar{\mathfrak{S}}$ is faithfully flat. If $\triangle$ is an ideal of $\bar{\mathfrak{S}}$, then with the same notations as before we have $\sigma(\triangle)\bar{\mathfrak{S}} = \triangle^{(p)}$.
Let C be a $\bar{\mathfrak{S}}$-module of finite type. Let $\mathfrak{a} \subset \bar{\mathfrak{S}}$ be the annihilator of C. Then $\mathfrak{a}^{(p)}$ is the annihilator of $C^{(\sigma)} = \bar{\mathfrak{S}} \otimes_{\sigma, \bar{\mathfrak{S}}} C$. This is clear for a monogenic module C. If we have more generators for C, then we can use the formula

$$\mathfrak{a}^{(p)} \cap \mathfrak{b}^{(p)} = (\mathfrak{a} \cap \mathfrak{b})^{(p)}$$

which holds for flat ring extensions in general.

We say that a power series $f \in \bar{\mathfrak{S}}$ of order u is normalized with respect to (T_1, T_2) if it contains T_1^u with a non-zero coefficient. This definition makes sense with respect to any regular system of parameters $\tilde{T}_1, \tilde{T}_2$ of $\bar{\mathfrak{S}}$.
We now assume that (a) holds and we show that (b) holds. Thus the $\bar{\mathfrak{S}}$-module C has finite length and the cokernel of $\varphi : C \to C^{(\sigma)}$ is annihilated by $\bar{h}$. Let k' be an infinite perfect field that contains k. Let $\bar{\mathfrak{S}}' := k'[[T_1, T_2]]$. To show that $C = 0$, it suffices to show that $\bar{\mathfrak{S}}' \otimes_{\bar{\mathfrak{S}}} C = 0$. Thus by replacing the role of k by the one of k', we can assume that k is infinite. This assumption implies that for almost all $\lambda \in k$, the power series $\bar{h}$ is normalized with respect to $(T_1, T_2 + \lambda T_1)$. By changing the regular system of parameters (T_1, T_2) in $\bar{\mathfrak{S}}$, we can assume that $\bar{h}$ is normalized with respect to (T_1, T_2). By the Weierstraß preparation theorem we can assume that $\bar{h}$ is a Weierstraß polynomial ([Bou], Chapter 7, Section 3, number 8). Thus we can write

$$\bar{h} = T_1^e + a_{e-1}(T_2)T_1^{e-1} + \ldots + a_1(T_2)T_1 + a_0(T_2),$$

where $a_0(T_2), \ldots, a_{e-1}(T_2) \in T_2 k[[T_2]]$.
We note that the assumption (a) implies that $e \leq 2p - 3$.
Let u be the minimal non-negative integer such that there exists a power series of the form $T_1^u + g \in \bar{\mathfrak{S}}$, with $g \in T_2\bar{\mathfrak{S}}$, for which we have $(T_1^u + g)C = 0$. By our assumptions, such a non-negative integer u exists.
We will show that the assumption that $C \neq 0$ leads to a contradiction. This assumption implies that $u \geq 1$. The annihilator $\mathfrak{a}$ of the module C has a set of generators of the following form:

$$T_1^{u_i} + g_i, (\text{with } i = 1, \ldots, l), \quad g_i \ (\text{with } i = l+1, \ldots, m),$$

where $u_i \geq u$ for $i = 1, \ldots, l$ and $g_i \in T_2\bar{\mathfrak{S}}$ for $i = 1, \ldots, m$.
As the cokernel of φ is annihilated by $\bar{h}$ we find that $(T_1^u + g)\bar{h}C^{(\sigma)} = 0$. As the annihilator of $C^{(\sigma)}$ is generated by the elements

$$T_1^{pu_i} + g_i^p \ (\text{with } i = 1, \ldots, l), \quad g_i^p \ (\text{with } i = l+1, \ldots, m), \tag{9}$$

we obtain the congruence

$$(T_1^u + g)\bar{h} \equiv 0 \mod (T_1^{up}, T_2^p). \tag{10}$$

We consider this congruence modulo T_2. We have $g \equiv 0 \mod (T_2)$ and $\bar{h} \equiv T_1^e \mod (T_2)$ because $\bar{h}$ is a Weierstraß polynomial. This proves that

$$T_1^u T_1^e \equiv 0 \mod (T_1^{up}).$$

But this implies that $u + e \geq up$. If $u \geq 2$, then $e \geq up - u \geq 2p - 2$ and this contradicts the inequality $e \leq 2p - 3$. Therefore we can assume that $u = 1$.
By replacing (T_1, T_2) with $(T_1 + g, T_2)$, without loss of generality we can assume that $T_1 C = 0$ and (cf. (10) and the equality $u = 1$) that

$$T_1\bar{h} \equiv 0 \mod \bar{\mathfrak{r}}^{(p)}.$$

This implies that up to a unit in $\bar{\mathfrak{S}}$ we can assume that $\bar{h}$ is of the form:

$$\bar{h} \equiv T_2^s T_1^{p-1} + \sum_{i=0}^{\infty} T_2^{i+p}\delta_i(T_1) \mod (T_1^p),$$

where $0 \leq s \leq p-2$ and where each $\delta_i \in k[T_1]$ has degree at most $p-2$.
Let now v be the smallest natural number such that $T_2^v C = 0$. Then the annihilator $\mathfrak{a}$ of C is generated by T_1, T_2^v and the annihilator $\mathfrak{a}^{(p)}$ of $C^{(\sigma)}$ is generated by T_1^p, T_2^{pv}. As the cokernel of φ is annihilated by $\bar{h}$, we find that $T_2^v \bar{h} C^{(\sigma)} = 0$. Thus we obtain the congruence

$$T_2^v(T_2^s T_1^{p-1} + \sum_{i=0}^{\infty} T_2^{i+p}\delta_i(T_1)) \equiv 0 \mod (T_1^p, T_2^{pv}).$$

But this implies $v + s \geq pv$. Thus $s \geq (p-1)v \geq p-1$ and (as $0 \leq s \leq p-2$) we reached a contradiction. Therefore $C = 0$ and thus (a) implies (b). □

Proposition 13 *We assume that $p \notin \mathfrak{m}^p$ (i.e., $e \leq p-1$). If $p \in \mathfrak{m}^{p-1}$, then we also assume that the ideal generated by the initial form of p in $\operatorname{gr} R$ is not a $(p-1)$-th power (thus $p > 2$).*
We consider a morphism $\alpha : (M_1, \varphi_1) \to (M_2, \varphi_2)$ of Breuil modules for the standard frame $\mathcal{L}$. Let $\mathfrak{p}$ be a prime ideal of R which contains p. We consider the $W(\kappa(\mathfrak{p})^{\mathrm{perf}})$-linear map obtained from α by base change

$$W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}}, \mathfrak{S}} M_1 \to W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}}, \mathfrak{S}} M_2. \tag{11}$$

Then the following two properties hold:

(a) If (11) is surjective, then the $\mathfrak{S}$-linear map $M_1 \to M_2$ is surjective.
(b) If (11) is injective, then the $\mathfrak{S}$-linear map $M_1 \to M_2$ is injective and its cokernel is a $\mathfrak{S}$-module of projective dimension at most 1.

Proof. We prove (a). We denote by $\tilde{\mathfrak{p}}$ the ideal of $\mathfrak{S}$ which corresponds to $\mathfrak{p}$ via the isomorphism $\mathfrak{S}/(E, p) \cong R/(p)$. It follows from the lemma of Nakayama that $(M_1)_{\tilde{\mathfrak{p}}} \to (M_2)_{\tilde{\mathfrak{p}}}$ is a surjection. Let us denote by (C, φ) the cokernel of α. We conclude that C is annihilated by an element $f \notin \tilde{\mathfrak{p}} \supset p\mathfrak{S}$. Therefore we conclude from Lemma 11 that $C = 0$. Thus (a) holds.
Part (b) follows from (a) by duality as it is compatible with taking fibres (6). Indeed for the last assertion it is enough to note that the kernel of the surjection $M_2^* \twoheadrightarrow M_1^*$ has clearly projective dimension at most 1. □

Remark. If $e = p-1$ and the ideal generated by the initial form of p in $\operatorname{gr} R$ is a $(p-1)$-th power, then the Proposition 13 is not true in general. This is so as there exist non-trivial homomorphisms $(\mathbb{Z}/p\mathbb{Z})_R \to \boldsymbol{\mu}_{p,R}$ for suitable such R's.

Proposition 14 *We assume that R has dimension $d = 2$ and that $h \in \mathfrak{S}$ does not belong to the ideal $(p, T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$ of $\mathfrak{S}$. Let $\alpha : (M_1, \varphi_1) \to (M_2, \varphi_2)$*

be a morphism of Breuil modules for the standard frame $\mathcal{L}$. We assume that for each prime ideal $\mathfrak{p}$ of R with $p \in \mathfrak{p} \neq \mathfrak{m}$, the $W(\kappa(\mathfrak{p})^{\mathrm{perf}})$-linear map obtained from α by base change

$$W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}},\mathfrak{S}} M_1 \to W(\kappa(\mathfrak{p})^{\mathrm{perf}}) \otimes_{\sigma\varkappa_{\mathfrak{p}},\mathfrak{S}} M_2 \tag{12}$$

is surjective (resp. is injective).
Then the $\mathfrak{S}$-linear map $M_1 \to M_2$ is surjective (resp. is injective and its cokernel is a $\mathfrak{S}$-module of projective dimension at most 1).

Proof. As in the last proof we only have to treat the case where the maps (12) are surjective. We consider the cokernel (C, φ) of α. As in the last proof we will argue that $C = 0$ but with the role of Lemma 11 being replaced by Lemma 12. It suffices to show that $\bar{C} := C/pC$ is zero. Let $\bar{\varphi} : \bar{C} \to \bar{C}^{(\sigma)}$ be the map induced naturally by φ.
Lemma 12 is applicable if we verify that $\bar{C}$ is a $\bar{\mathfrak{S}}$-module of finite length.
We denote by $\bar{\mathfrak{p}}$ the ideal of $\bar{\mathfrak{S}} = \mathfrak{S}/p\mathfrak{S}$ which corresponds to $\mathfrak{p}$ via the isomorphism $\bar{\mathfrak{S}}/(\bar{h}) \cong R/pR$. It follows from (12) by the lemma of Nakayama that for each prime ideal $\bar{\mathfrak{p}} \supset \bar{h}\bar{\mathfrak{S}}$ different from the maximal ideal of $\bar{\mathfrak{S}}$ the maps $\alpha_{\mathfrak{p}} : (M_1)_{\bar{\mathfrak{p}}} \to (M_2)_{\bar{\mathfrak{p}}}$ are surjective. Using this one constructs inductively a regular sequence $f_1, \ldots, f_{d-1}, \bar{h}$ in the ring $\bar{\mathfrak{S}}$ such that the elements $f_1, \ldots, f_{d-1}$ annihilate $\bar{C}$. As $\bar{C}$ is a finitely generated module over the 1-dimensional local ring $\bar{\mathfrak{S}}/(f_1, \ldots, f_{d-1})$, we get that $\bar{C}[1/\bar{h}]$ is a module of finite length over the regular ring $A = \bar{\mathfrak{S}}[1/\bar{h}]$. If we can show that $\bar{C}[1/\bar{h}] = 0$, then it follows that $\bar{C}$ is of finite length.
As we are in characteristic p, the Frobenius σ acts on the principal ideal domain $A = \bar{\mathfrak{S}}[1/\bar{h}]$. By the definition of a Breuil module the maps $\varphi_i[1/\bar{h}]$ for $i = 1, 2$ become isomorphisms. Therefore φ gives birth to an isomorphism:

$$\bar{\varphi}[1/\bar{h}] : \bar{C}[1/\bar{h}] \to (\bar{C}[1/\bar{h}])^{(\sigma)}. \tag{13}$$

As A is regular of dimension $d-1$, for each A-module $\ddagger$ of finite length we have

$$\mathrm{length}\, \ddagger^{(\sigma)} = p^{d-1}\, \mathrm{length}\, \ddagger.$$

We see that the isomorphism (13) is only possible if $\bar{C}[1/\bar{h}] = 0$. Thus $\bar{C}$ has finite length and therefore from Lemma 12 we get that $\bar{C} = 0$. This implies that $C = 0$. □

4 Extending epimorphisms and monomorphisms

In this section let R be a regular local ring of mixed characteristic $(0, p)$ with maximal ideal $\mathfrak{m}$ and residue class field k. Let K be the field of fractions of R.

4.1 Complements on Raynaud's work

We first reprove Raynaud's result [R2], Corollary 3.3.6 by the methods of the previous sections. We state it in a slightly different form.

Proposition 15 *We assume that $p \notin \mathfrak{m}^{p-1}$ (thus $p > 2$). Let H_1 and H_2 be finite flat group schemes over* $\operatorname{Spec} R$. *Let $\beta : H_1 \to H_2$ be a homomorphism, which induces an epimorphism (resp. monomorphism) $H_{1,K} \to H_{2,K}$ between generic fibres. Then β is an epimorphism (resp. monomorphism).*

Proof. We prove only the statement about epimorphisms because the case of a monomorphism follows by Cartier duality. It is enough to show that the homomorphism $H_1 \to H_2$ is flat. By the fibre criterion of flatness it is enough to show that the homomorphism $\beta_k : H_{1,k} \to H_{2,k}$ between special fibres is an epimorphism. To see this we can assume that R is a complete local ring with algebraically closed residue class field k.
We write $R \cong \mathfrak{S}/(p-h)$, with $\mathfrak{S} = W(k)[[T_1, \ldots, T_d]]$. Then the reduction $\bar{h} \in k[[T_1, \ldots, T_d]]$ of h modulo p is a power series of order $e < p-1$. By Noether normalization theorem we can assume that $\bar{h}$ contains the monom T_1^e. By replacing R with $R/(T_2, \ldots, T_d)$, we can assume that R is one-dimensional. We consider the morphism

$$(M_1, \varphi_1) \to (M_2, \varphi_2)$$

of Breuil modules associated to β. Let (C, φ) be its cokernel. Let $\bar{C} := C/C_0$, where C_0 is the $\mathfrak{S}$-submodule of C whose elements are annihilated by a power of the maximal ideal $\mathfrak{r}$ of $\mathfrak{S}$. The $\mathfrak{S}$-linear map φ factors as

$$\bar{\varphi} : \bar{C} \to \mathfrak{S} \otimes_{\sigma, \mathfrak{S}} \bar{C}$$

and the cokernel of $\bar{\varphi}$ is annihilated by $\bar{h}$. The maximal ideal $\mathfrak{r}$ of $\mathfrak{S}$ is not associated to $\mathfrak{S} \otimes_{\sigma, \mathfrak{S}} \bar{C}$. Thus either $\bar{C} = 0$ or $\operatorname{depth} \bar{C} \geq 1$. Therefore the $\mathfrak{S}$-module $\bar{C}$ is of projective dimension at most 1. As $\bar{C}$ is annihilated by a power of p, we conclude that $(\bar{C}, \bar{\varphi})$ is the Breuil module of a finite flat group scheme D over $\operatorname{Spec} R$. We have induced homomorphisms

$$H_1 \to H_2 \to D.$$

The composition of them is zero and the second homomorphism is an epimorphism because it is so after base change to k. As $H_{1,K} \twoheadrightarrow H_{2,K}$ is an epimorphism we conclude that $D_K = 0$. But then $D = 0$ and the Breuil module $(\bar{C}, \bar{\varphi})$ is zero as well. We conclude by Lemma 11 that $C = 0$. □

The next proposition is proved in [R2], Remark 3.3.5 in the case of biconnected finite flat group schemes H and D.

Proposition 16 *Let R be a discrete valuation ring of mixed characteristic $(0, p)$ and index of ramification $p-1$; we have $K = R[1/p]$. Let $\beta : H \to D$ be a homomorphism of residually connected finite flat group schemes over* $\operatorname{Spec} R$ *which induces an isomorphism (resp. epimorphism) over* $\operatorname{Spec} K$.
Then β is an isomorphism (resp. epimorphism).

Proof. It is enough to show the statement about isomorphisms. Indeed, assume that β_K is an epimorphism. Consider the schematic closure H_1 of the kernel of β_K in H. Then $H/H_1 \to D$ is an isomorphism.
Therefore we can assume that β_K is an isomorphism. By extending R we can assume that R is complete and that k is algebraically closed. By considering the Cartier dual homomorphism $\beta^{\mathrm{t}} : D^{\mathrm{t}} \to H^{\mathrm{t}}$ one easily reduces the problem to the case when H is biconnected. As the case when D is also biconnected is known (cf. [R2], Remark 3.3.5), one can easily reduce to the case when D is of multiplicative type. Then D contains $\boldsymbol{\mu}_{p,R}$ as a closed subgroup scheme. We consider the schematic closure H_1 of $\boldsymbol{\mu}_{p,K}$ in H. Using an induction on the order of H it is enough to show that the natural homomorphism $\beta_1 : H_1 \to \boldsymbol{\mu}_{p,R}$ is an isomorphism. This follows from [R2], Proposition 3.3.2 3°. For the sake of completeness we reprove this in the spirit of the paper.
We write $R = \mathfrak{S}/(E)$, where $E \in \mathfrak{S} = W(k)[[T]]$ is an Eisenstein polynomial of degree $e = p-1$. The Breuil window of the p-divisible group $\boldsymbol{\mu}_{p^\infty,R}$ is given by

$$\begin{array}{ccc} \mathfrak{S} & \to & \mathfrak{S}^{(\sigma)} \cong \mathfrak{S} \\ f & \mapsto & Ef. \end{array}$$

The Breuil module (N,τ) of $\boldsymbol{\mu}_{p,R}$ is the kernel of the multiplication by p : $\boldsymbol{\mu}_{p^\infty,R} \to \boldsymbol{\mu}_{p^\infty,R}$ and therefore it can be identified with

$$\begin{array}{ccc} N = k[[T]] & \to & N^{(\sigma)} = k[[T]]^{(\sigma)} \cong k[[T]] \\ f & \mapsto & T^e f. \end{array}$$

Let (M,φ) be the Breuil module of H_1. As H_1 is of height 1 we can identify $M = k[[T]]$. Then $\varphi : M \to M^{(\sigma)} \cong M$ is the multiplication by a power series $g \in k[[T]]$ of order $\mathrm{ord}(g) \le e = p-1$. To the homomorphism $\beta_1 : H_1 \to \boldsymbol{\mu}_{p,R}$ corresponds a morphism $\alpha_1 : (M,\varphi) \to (N,\tau)$ that maps $1 \in M$ to some element $a \in N$. We get a commutative diagram:

$$\begin{array}{ccc} k[[T]] & \xrightarrow{\;a\;} & k[[T]] \\ {\scriptstyle g}\downarrow & & \downarrow{\scriptstyle T^e} \\ k[[T]] & \xrightarrow{\;a^p\;} & k[[T]]. \end{array}$$

We obtain the equation $ga = a^pT^{p-1}$. As $a \neq 0$ this is only possible if

$$\mathrm{ord}(g) = (p-1)(\mathrm{ord}(a)+1).$$

As $\mathrm{ord}(g) \le p-1$, we get that $\mathrm{ord}(a) = 0$ and $\mathrm{ord}(g) = p-1$. As $\mathrm{ord}(a) = 0$, both α_1 and β_1 are isomorphisms. Thus $\beta : H \to D$ is an isomorphism. □

4.2 Basic extension properties

The next three results will be proved for $p = 2$ under certain residually connectivity assumptions. But in Subsection 4.3 below we will show how these results hold under no residually connectivity assumptions even if $p = 2$.

Proposition 17 *We assume that* $\dim R \geq 2$, *that* $p \notin \mathfrak{m}^p$, *and that the initial form of* p *in* $\operatorname{gr} R$ *generates an ideal which is not a* $(p-1)$*-th power. Let* $\beta : H_1 \to H_2$ *be a homomorphism of finite flat group schemes over* $\operatorname{Spec} R$ *which induces an epimorphism (resp. a monomorphism) over* $\operatorname{Spec} K$. *If* $p = 2$, *we assume as well that* H_1 *and* H_2 *(resp. that the Cartier duals of* H_1 *and* H_2*) are residually connected.*
Then β *is an epimorphism (resp. a monomorphism).*

Proof. As before we can assume that R is a complete regular local ring. We can also restrict our attention to the case of epimorphisms.
By Proposition 15 we can assume that $p \in \mathfrak{m}^{p-1}$. Let $\mathfrak{p}$ be a minimal prime ideal which contains p. We show that the assumption that $p \in \mathfrak{p}^{p-1}$ leads to a contradiction. Then we can write $p = uf^{p-1}$, where $u, f \in R$ and f is a generator of the prime ideal $\mathfrak{p}$. It follows from our assumptions that $u \notin \mathfrak{m}$ and that $f \in \mathfrak{m} \setminus \mathfrak{m}^2$. Therefore the initial form of p in $\operatorname{gr} R$ generates an ideal which is a $(p-1)$-th power. Contradiction.
We first consider the case when k is perfect. Let $\alpha : (M_1, \varphi_1) \to (M_2, \varphi_2)$ denote also the morphism of Breuil modules associated to $\beta : H_1 \to H_2$. As $p \notin \mathfrak{p}^{p-1}$, we can apply Proposition 15 to the ring $R_{\mathfrak{p}}$. It follows that β induces an epimorphism over the spectrum of the residue class field $\kappa(\mathfrak{p})$ of $\mathfrak{p}$ and thus also of its perfect hull $\kappa(\mathfrak{p})^{\mathrm{perf}}$. From this and the end of Section 2 we get that the hypotheses of Proposition 13 hold for α. We conclude that α is an epimorphism and thus β is also an epimorphism.
Let $R \to R'$ be a faithfully flat extension of noetherian local rings, such that $\mathfrak{m}R'$ is the maximal ideal of R' and the extension of residue class fields $k \hookrightarrow k'$ is radical. We consider the homomorphism of polynomial rings $\operatorname{gr} R \to \operatorname{gr} R'$. As $\operatorname{gr} R$ and $\operatorname{gr} R'$ are unique factorization domains, it is easy to see that the condition that the initial form of p is not a $(p-1)$-th power is stable by the extension $R \to R'$. But β is an epimorphism if and only if $\beta_{R'}$ is so. Therefore we can assume that the residue class field of R is perfect and this case was already proved. □

Proposition 18 *We assume that* $\dim R = 2$. *Let* $U = \operatorname{Spec} R \setminus \{\mathfrak{m}\}$. *We also assume that the following technical condition holds:*

(*) *there exists a faithfully flat local* R*-algebra* $\hat{R}$ *which is complete, which has an algebraically closed residue class field* k, *and which has a presentation* $\hat{R} = \mathfrak{S}/(p-h)$ *where* $\mathfrak{S} = W(k)[[T_1, T_2]]$ *and where* $h \in (T_1, T_2)$ *does not belong to the ideal* $(p, T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$.

Let $\beta : H_1 \to H_2$ *be a homomorphism of finite flat group schemes over* $\operatorname{Spec} R$. *We also assume that for each geometric point* $\operatorname{Spec} L \to U$ *such that* L *has characteristic* p *the homomorphism* β_L *is an epimorphism (resp. a monomorphism); thus* $\beta_U : H_{1,U} \to H_{2,U}$ *is an epimorphism (resp. a monomorphism). If* $p = 2$, *we assume that* H_1 *and* H_2 *(resp. that the Cartier duals of* H_1 *and* H_2*) are residually connected.*
Then β *is an epimorphism (resp. a monomorphism).*

Proof. We have $\dim \hat{R}/\mathfrak{m}\hat{R} = 0$ and thus $\mathrm{Spec}(\hat{R}) \setminus (\mathrm{Spec}(\hat{R}) \times_{\mathrm{Spec}\, R} U)$ is the closed point of $\mathrm{Spec}(\hat{R})$. Based on this we can assume that $R = \hat{R}$. Thus the proposition follows from Proposition 14 in the same way Proposition 17 followed from Propositions 15 and 13. □

Corollary 19 *We assume that the assumptions on R of either Proposition 17 or Proposition 18 are satisfied (thus $\dim R \geq 2$). We consider a complex*

$$0 \to H_1 \to H_2 \to H_3 \to 0$$

of finite flat group schemes over $\mathrm{Spec}\, R$ whose restriction to $U = \mathrm{Spec}\, R \backslash \{\mathfrak{m}\}$ is a short exact sequence. If $p = 2$, then we assume that H_2 and H_3 are residually connected. Then $0 \to H_1 \to H_2 \to H_3 \to 0$ is a short exact sequence.

Proof. Propositions 17 and 18 imply that $H_2 \to H_3$ is an epimorphism. Its kernel is a finite flat group scheme isomorphic to H_1 over U and thus (as we have $\dim R \geq 2$) it is isomorphic to H_1. □

4.3 Dévissage properties

In this subsection we explain how one can get the results of Subsection 4.2 under no residually connectivity assumptions for $p = 2$.

We assume that $\dim R = 2$ and that p is arbitrary. Let $U = \mathrm{Spec}\, R \setminus \{\mathfrak{m}\}$. Let $\mathcal{V}$ be a locally free $\mathcal{O}_U$-module of finite rank over U. The R-module $H^0(U, \mathcal{V})$ is free of finite rank. Using this it is easy to see that each finite flat group scheme over U extends uniquely to a finite flat group scheme over $\mathrm{Spec}\, R$. This is clearly an equivalence between the category of finite flat group schemes over U and the category of finite flat group schemes over $\mathrm{Spec}\, R$. The same holds if we restrict to finite flat group schemes annihilated by p.

Next we also assume that R is complete. Each finite flat group scheme H over $\mathrm{Spec}\, R$ is canonically an extension

$$0 \to H^{\circ} \to H \to H^{\text{ét}} \to 0,$$

where H° is connected and $H^{\text{ét}}$ is étale over $\mathrm{Spec}\, R$. In particular a homomorphism from a connected finite flat group scheme over $\mathrm{Spec}\, R$ to an étale finite flat group scheme over $\mathrm{Spec}\, R$ is zero. From this one easily checks that if $H_1 \to H_2$ is a homomorphism of finite flat group schemes over $\mathrm{Spec}\, R$ which is an epimorphism over U and if H_1 is connected, then H_2 is connected as well.

Lemma 20 *We assume that $\dim R = 2$ and that R is complete. Then the following four statements are equivalent:*

(a) *Each short exact sequence of finite flat group schemes over U extends uniquely to a short exact sequence of finite flat group schemes over* $\mathrm{Spec}\, R$.

(b) *Let* H_1 *and* H_2 *be connected finite flat group schemes over* $\operatorname{Spec} R$. *A homomorphism* $H_1 \to H_2$ *over* $\operatorname{Spec} R$ *is an epimorphism if its restriction to* U *is an epimorphism.*

(c) *Let* H_1 *and* H_2 *be connected finite flat group schemes over* $\operatorname{Spec} R$ *which are annihilated by* p. *A homomorphism* $H_1 \to H_2$ *over* $\operatorname{Spec} R$ *is an epimorphism if its restriction to* U *is an epimorphism.*

(d) *The regular ring* R *is* p*-quasi-healthy.*

Proof. It is clear that (a) implies (b). We show that (b) implies (a). Let

$$0 \to H_1 \to H_2 \to H_3 \to 0$$

be a complex of finite flat group schemes over $\operatorname{Spec} R$ whose restriction to U is a short exact sequence. It suffices to show that $\beta : H_1 \to H_2$ is a monomorphism. Indeed, in this case we can form the quotient group scheme H_2/H_1 and the homomorphism $H_2/H_1 \to H_3$ is an isomorphism as its restriction to U is so.
We check that the homomorphism

$$\beta^\circ : H_1^\circ \to H_2^\circ$$

is a monomorphism. Let H_4 be the finite flat group scheme over R whose restriction to U is $H_{2,U}^\circ/H_{1,U}^\circ$. We have a complex $0 \to H_1^\circ \to H_2^\circ \to H_4 \to 0$ whose restriction to U is exact. We conclude that H_4 is connected. Thus we have an epimorphism $H_2^\circ \twoheadrightarrow H_4$ (as we are assuming that (b) holds) whose kernel is H_1°. Therefore (b) implies that β° is a monomorphism.
As β° is a monomorphism, it suffices to show that the induced homomorphism $\bar{\beta} : H_1/H_1^\circ \to H_2/H_1^\circ$ is a monomorphism. In other words, without loss of generality we can assume that $H_1 = H_1^{\text{ét}}$ is étale.
Let H_1'' be the kernel of $H_2^{\text{ét}} \to H_3^{\text{ét}}$; it is a finite étale group scheme over $\operatorname{Spec} R$. Let H_1' be the kernel of $H_1 \to H_1''$. It suffices to show that $H_1' \to H_2^\circ$ is a monomorphism. Therefore we can also assume that H_2 is connected. This implies that H_3 is connected. As we are assuming that (b) holds, $H_2 \to H_3$ is an epimorphism. Its kernel is H_1 and therefore $\beta : H_1 \to H_2$ is a monomorphism. Thus (b) implies (a).
We show that (c) implies (b). The last argument shows that a short exact sequence of finite flat group schemes over U annihilated by p extends to a short exact sequence of finite flat group schemes over $\operatorname{Spec} R$. We start with a homomorphism $H_2 \to H_3$ between connected finite flat group schemes over $\operatorname{Spec} R$ which induces an epimorphism over U. We extend the kernel of $H_{2,U} \to H_{3,U}$ to a finite flat group scheme H_1 over $\operatorname{Spec} R$. Then we find a complex

$$0 \to H_1 \to H_2 \to H_3 \to 0$$

whose restriction to U is a short exact sequence. To show that $H_2 \to H_3$ is an epimorphism it is equivalent to show that $H_1 \to H_2$ is a monomorphism.

As $H_{1,U}$ has a composition series whose factors are annihilated by p, we easily reduce to the case where H_1 is annihilated by p. We embed H_2 into a p-divisible group G over $\operatorname{Spec} R$. To check that $H_1 \to H_2$ is a monomorphism, it suffices to show that $H_1 \to G[p]$ is a monomorphism. But this follows from the second sentence of this paragraph.
It is clear that (a) implies (d). We are left to show that (d) implies (c). It suffices to show that a homomorphism $\beta : H_1 \to H_2$ of finite flat group schemes over $\operatorname{Spec} R$ annihilated by p is a monomorphism if its restriction $\beta_U : H_{1,U} \to H_{2,U}$ is a monomorphism. We embed H_2 into a p-divisible group G over $\operatorname{Spec} R$. The quotient $G_U/H_{1,U}$ is a p-divisible group over U which extends to a p-divisible group G' over $\operatorname{Spec} R$ (as we are assuming that (d) holds). The isogeny $G_U \to G'_U$ extends to an isogeny $G \to G'$. Its kernel is a finite flat group scheme and therefore isomorphic to H_1. We obtain a monomorphism $H_1 \to G$. Thus $\beta : H_1 \to H_2$ is a monomorphism, i.e. (d) implies (c). □

Corollary 21 *Propositions 17 and 18 (and thus implicitly Corollary 19) hold without any residually connectivity assumption for $p = 2$.*

Proof. We can assume that R is complete. By considering an epimorphism $R \twoheadrightarrow R'$ with R' regular of dimension 2, we can also assume that $\dim R = 2$. Based on Lemma 20, it suffices to prove Propositions 17 and 18 in the case when connected finite flat group schemes are involved. But this case was already proved in Subsection 4.2. This also shows that for $p \geq 3$ we can restrict to the connected case and avoid to apply Proposition 10 for nonconnected p-divisible groups. □

Corollary 22 *We assume that k is perfect and that $R = W(k)[[T_1, T_2]]/(p - h)$ with $h \in (T_1, T_2)$. Let $\bar{h} \in k[[T_1, T_2]]$ be the reduction of h modulo p. Then the fact that R is or is not p-quasi-healthy depends only on the orbit of the ideal $(\bar{h})$ of $k[[T_1, T_2]]$ under automorphisms of $k[[T_1, T_2]]$.*

Proof. The category of Breuil modules associated to connected finite flat group schemes over $\operatorname{Spec} R$ annihilated by p is equivalent to the category of pairs (M, φ), where M is a free $k[[T_1, T_2]]$-module of finite rank and where $\varphi : M \to M^{(\sigma)}$ is a $k[[T_1, T_2]]$-linear map whose cokernel is annihilated by $\bar{h}$ and whose reduction modulo the ideal (T_1, T_2) is nilpotent in the natural sense. The last category depends only on the orbit of $(\bar{h})$ under automorphisms of $k[[T_1, T_2]]$. The corollary follows from the last two sentences and the equivalence of (c) and (d) in Lemma 20. □

4.4 The p-quasi-healthy part of Theorem 3

In this subsection we show that if R is as in Theorem 3 for $d = 2$, then R is p-quasi-healthy. It follows from the definition of a p-divisible group and the uniqueness part of the first paragraph of Subsection 4.3, that it is enough to show that a complex $0 \to H_1 \to H_2 \to H_3 \to 0$ of finite flat group schemes over $\operatorname{Spec} R$ is a short exact sequence if its restriction to $\operatorname{Spec} R \setminus \{\mathfrak{m}\}$ is a short exact sequence. This is a local statement in the faithfully flat topology of $\operatorname{Spec} R$ and thus to check it we can assume that $R = \hat{R} = W(k)[[T_1, T_2]/(p-h)$ with $h \in (T_1, T_2)$ but $h \notin (p, T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$. By Lemma 20 we can assume that H_2 and H_3 are connected. Thus $0 \to H_1 \to H_2 \to H_3 \to 0$ is a short exact sequence, cf. Corollary 19. □

5 Extending abelian schemes

Proposition 23 *Let R be a regular local ring of mixed characteristic $(0, p)$.*

(a) Let $U = \operatorname{Spec} R \setminus \{\mathfrak{m}\}$, where $\mathfrak{m}$ is the maximal ideal of R. Let $\breve{A}$ be an abelian scheme over U. If the p-divisible group of $\breve{A}$ extends to a p-divisible group over $\operatorname{Spec} R$, then $\breve{A}$ extends uniquely to an abelian scheme A over $\operatorname{Spec} R$.

(b) If R is p-quasi-healthy, then R is quasi-healthy.

Proof. The uniqueness part of (a) is well known (cf. [R1], Chapter IX, Corollary 1.4). Part (a) is a particular case of either proof of [V2], Proposition 4.1 (see remark that starts the proof) or [V2], Remark 4.2. Part (b) follows from (a). □

Lemma 24 *Let $S \twoheadrightarrow R$ be a ring epimorphism between local noetherian rings whose kernel is an ideal $\mathfrak{a}$ with $\mathfrak{a}^2 = 0$ and $\operatorname{depth}_R \mathfrak{a} \geq 2$. We assume that $\operatorname{depth} R \geq 2$ and that R is quasi-healthy. Then S is quasi-healthy as well.*

Proof. Let $\mathfrak{m}$ and $\mathfrak{n}$ be the maximal ideals of R and S (respectively). We set $U = \operatorname{Spec} R \setminus \{\mathfrak{m}\}$ and $V = \operatorname{Spec} S \setminus \{\mathfrak{n}\}$.
Let $\breve{B}$ be an abelian scheme over V and let $\breve{A}$ be its reduction over U. Then $\breve{A}$ extends uniquely to an abelian scheme A over $\operatorname{Spec} R$. Let $\pi : A \twoheadrightarrow \operatorname{Spec} R$ be the projection. It is well-known that the set of liftings of A with respect to $\operatorname{Spec} R \hookrightarrow \operatorname{Spec} S$ is a trivial torsor under the group $H^0(\operatorname{Spec} R, R^1\pi_*\underline{\operatorname{Hom}}(\Omega_{A/R}, \mathfrak{a}))$ and that the set of liftings of $\breve{A}$ with respect to $V \twoheadrightarrow U$ is a trivial torsor under the group $H^0(U, R^1\pi_*\underline{\operatorname{Hom}}(\Omega_{A/R}, \mathfrak{a}))$. As $\operatorname{depth}_R \mathfrak{a} \geq 2$, the last two groups are equal. Thus there exists a unique abelian scheme B over $\operatorname{Spec} S$ which lifts A and whose restriction to V is $\breve{B}$. □

Proposition 25 *Let S be a complete noetherian local ring of mixed characteristic $(0, p)$. Let $S \twoheadrightarrow R$ be a ring epimorphism with kernel $\mathfrak{a}$ (thus R is a complete noetherian local ring). We assume that there exists a sequence of ideals*

$$\mathfrak{a} = \mathfrak{a}_0 \supset \mathfrak{a}_1 \supset \dots$$

such that the intersection of these ideals is 0 and for all $i \geq 0$ we have $\mathfrak{a}_i^2 \subset \mathfrak{a}_{i+1}$ and $\operatorname{depth}_S \mathfrak{a}_i/\mathfrak{a}_{i+1} \geq 2$. We also assume that $\operatorname{depth} R \geq 2$ and that R is quasi-healthy. Let $\mathfrak{n}$ be the maximal ideal of S. Let $V := \operatorname{Spec} S \setminus \{\mathfrak{n}\}$.

(a) Then each abelian scheme over V that has a polarization extends to an abelian scheme over $\mathrm{Spec}\, S$.

(b) We assume that S is integral and geometrically unibranch (like S is normal). Then S is quasi-healthy.

Proof. By a well-known theorem we have $S = \lim\limits_{\leftarrow} S/\mathfrak{a}_i$.

For (b) (resp. (a)) we have to show that each abelian scheme $\breve{A}$ (resp. each abelian scheme $\breve{A}$ that has a polarization $\lambda_{\breve{A}}$) over V extends to an abelian scheme over $\mathrm{Spec}\, S$. We write $U_i = (\mathrm{Spec}\, S/\mathfrak{a}_i) \setminus \{\mathfrak{n}\}$. The topological space underlying U_i is independent of i and it will be denoted by U. It is easy to see that $\mathrm{depth}\, S/\mathfrak{a}_i \geq 2$. By Lemma 24 the ring $S/\mathfrak{a}_i$ is quasi-healthy. We denote by $\breve{A}_i$ the base change of $\breve{A}$ to U_i. Then $\breve{A}_i$ extends uniquely to an abelian scheme A_i over $\mathrm{Spec}\, S/\mathfrak{a}_i$. If S is integral and geometrically unibranch, then from [R1], Chapter XI, Theorem 1.4 we get that $\breve{A}$ is projective over V. Thus from now on we can assume that there exists a polarization $\lambda_{\breve{A}}$ of $\breve{A}$ and we will not anymore differentiate between parts (a) and (b).
From the uniqueness of A_i we easily get that the reduction of $\lambda_{\breve{A}}$ modulo $\mathfrak{a}_i$ extends uniquely to a polarization λ_{A_i} of A_i (this also follows from [R1], Chapter IX, Corollary 1.4). We get that the A_i's inherit a compatible system of polarizations. From this and the algebraization theorem of Grothendieck, we get that there exists an abelian scheme A over $\mathrm{Spec}\, S$ which lifts the A_i's. Next we will prove that the p-divisible group G of A restricts over V to the p-divisible group $\breve{G}$ of $\breve{A}$. This implies that $\breve{A}$ extends to an abelian scheme over $\mathrm{Spec}\, S$ (cf. Proposition 23 (a)) which is then necessarily isomorphic to A. Let $G_i[m]$ be the kernel of the multiplication by $p^m : A_i \to A_i$, and let $G[m]$ be the kernel of the multiplication by $p^m : A \to A$.
Let $C_i[m]$ be the $S/\mathfrak{a}_i$-algebra of global functions on $G_i[m]$. Then $B[m] = \lim\limits_{\leftarrow} C_i[m]$ is the S-algebra of global functions on $G[m]$.

We write $\underline{\mathrm{Spec}}\, \breve{\mathcal{C}}[m] = \breve{G}[m]$, where $\breve{\mathcal{C}}[m]$ is a finite $\mathcal{O}_{\breve{G}[m]}$-algebra. We have a natural homomorphism:

$$H^0(V, \breve{\mathcal{C}}[m]) \to H^0(U, (C_i[m])^{\sim}) = C_i[m].$$

Here $(C_i[m])^{\sim}$ is the restriction to U of the $\mathcal{O}_{\mathrm{Spec}\, S/\mathfrak{a}_i}$-algebra associated to $C_i[m]$. The last equality follows from the fact that $\mathrm{depth}\, S/\mathfrak{a}_i \geq 2$. This gives birth to an S-algebra homomorphism

$$H^0(V, \breve{\mathcal{C}}[m]) \to B[m].$$

If we restrict it to a homomorphism between $\mathcal{O}_V$-algebras we obtain a homomorphism of finite flat group schemes over V

$$G[m]_V \to \breve{G}[m]$$

and thus a homomorphism of corresponding p-divisible groups $G_V \to \breve{G}$ over V. By construction this is an isomorphism if we restrict it to U. As V is connected, from the following proposition we conclude that $G_V \to \breve{G}$ is an isomorphism. □

Proposition 26 *Let $\beta : G \to G'$ be a homomorphism of p-divisible groups over a noetherian scheme X. Then the set Y of points $x \in X$ such that β_x is an isomorphism is open and closed in X. Moreover β_Y is an isomorphism.*

Proof. It is clear that β is an isomorphism if and only if $\beta[1] : G[1] \to G'[1]$ is an isomorphism. Therefore the subfunctor of X defined by the condition that β_Y is an isomorphism is representable by an open subscheme $Z \subset X$.
By the theorems of Tate and de Jong on extensions of homomorphisms between p-divisible groups, we get that the valuative criterion of properness holds for $Z \to X$. Thus Z is as well closed in X and therefore we can take $Y = Z$. □

5.1 Counterexample for the p-quasi-healthy context

Lemma 24 does not hold for the p-quasi-healthy context even in the simplest cases. Here is an elementary counterexample. We take $R = W(k)[[T_1]]$. From Subsection 4.4 we get that R is p-quasi-healthy. We take $S = R[T_2]/(T_2^2)$. Let $V := \operatorname{Spec} S \setminus \{\mathfrak{n}\}$, where $\mathfrak{n}$ is the maximal ideal of S. Let $\mathcal{O} := R_{(T_1)}$; we have a natural identification $V = \operatorname{Spec} S[\frac{1}{T_1}] \cup \operatorname{Spec} \mathcal{O}[T_2]/(T_2^2)$.
Let $\mathcal{E}_k$ be an elliptic curve over $\operatorname{Spec} k$. We can identify the formal deformation space of $\mathcal{E}_k$ with $\operatorname{Spf} R$. Let $\mathcal{E}$ be the elliptic curve over $\operatorname{Spec} R$ which is the algebraization of the uni-versal elliptic curve over $\operatorname{Spf} R$. Let $\iota_1 : R \hookrightarrow S[\frac{1}{T_1}]$ be the $W(k)$-monomorphism that maps T_1 to $T_1 + T_2T_1^{-1}$; it lifts the natural $W(k)$-monomorphism $R \hookrightarrow R[\frac{1}{T_1}]$. The $W(k)$-monomorphism ι_1 gives birth to an elliptic curve $\mathcal{E}_1$ over $\operatorname{Spec} S[\frac{1}{T_1}]$ whose restriction to $\operatorname{Spec} S[\frac{1}{T_1}]/(T_2) = \operatorname{Spec} R[\frac{1}{T_1}]$ extends to the elliptic curve $\mathcal{E}$ over $\operatorname{Spec} R$.
We check that the assumption that $\mathcal{E}_1$ extends to an elliptic curve $\mathcal{E}_V$ over V leads to a contradiction. To $\mathcal{E}_V$ and $\mathcal{E}_U$ correspond morphisms $U \to V \to \mathbb{A}^1$, where $\mathbb{A}^1$ is the j-line over $\operatorname{Spec} W(k)$. As the topological spaces of U and V are equal, we get that we have a natural factorization $U \to V \to \operatorname{Spec} R \to \mathbb{A}^1$, where we identify $\operatorname{Spec} R$ with the completion of $\mathbb{A}^1$ at its k-valued point defined by $\mathcal{E}_k$. As $S = H^0(V, \mathcal{O}_V)$, the image of ι_1 is contained in S. Contradiction.
But the p-divisible group $\mathcal{G}_1$ of $\mathcal{E}_1$ extends to a p-divisible group $\mathcal{G}_V$ over V. This is so as each p-divisible group over $\operatorname{Spec} \mathcal{O}$ extends uniquely to an étale p-divisible group over $\operatorname{Spec} \mathcal{O}[T_2]/(T_2^2)$.
Finally we check that the assumption that $\mathcal{G}_V$ extends to a p-divisible group $\mathcal{G}_2$ over $\operatorname{Spec} S$ leads to a contradiction. Let $\mathcal{E}_2$ be the elliptic curve over $\operatorname{Spec} S$ which lifts $\mathcal{E}$ and whose p-divisible group is $\mathcal{G}_2$. Let $\iota_2 : R \to S$ be the $W(k)$-homomorphism that defines $\mathcal{E}_2$. We check that the resulting two $W(k)$-homomorphisms $\iota_1, \iota_2 : R \to S[\frac{1}{T_1}]$ are equal. It suffices to show that their composites $\iota_3, \iota_4 : R \to \widehat{S_{(p)}}$ with the natural $W(k)$-monomorphism $S[\frac{1}{T_1}] \hookrightarrow \widehat{S_{(p)}} = \widehat{R_{(p)}}[T_2]/(T_2^2)$ are equal (here $\widehat{\triangle}$ denotes the completion of the local ring $\triangle$). But this follows from Serre–Tate deformation theory and the fact that the

composites $\iota_5, \iota_6 : R \to \widehat{R_{(p)}}$ of ι_3, ι_4 with the $W(k)$-epimorphism $\widehat{S_{(p)}} \twoheadrightarrow \widehat{R_{(p)}}$, are equal. As the two $W(k)$-homomorphisms $\iota_1, \iota_2 : R \to S[\frac{1}{T_1}]$ are equal, the image of ι_1 is contained in S. Contradiction.
We conclude that S is not p-quasi-healthy. A similar argument shows that for all $n \geq 2$, the ring $R[T_2]/(T_2^n)$ is not p-quasi-healthy.
This counterexample disproves the claims on [FC], top of p. 184 on torsors of liftings of p-divisible groups.

5.2 Proofs of Theorem 3 and Corollary 4

Let $\mathfrak{m}$ be the maximal ideal of R. Let $U = \operatorname{Spec} R \setminus \{\mathfrak{m}\}$. Let $d = \dim R$.
We prove Theorem 3. We first assume that $d = 2$. It is enough to show that R is p-quasi-healthy, cf. Proposition 23 (b). But this follows from Subsection 4.4. We next assume that $d \geq 3$. We have to show that each abelian scheme over U extends uniquely to an abelian scheme over $\operatorname{Spec} R$. This is a local statement in the faithfully flat topology of $\operatorname{Spec} R$ and thus to check it we can assume that $R = \hat{R}$ is complete with algebraically closed residue class field k. We have an epimorphism $R \twoheadrightarrow W(k)[[T_1, T_2]]/(p - h)$ where h is a power series in the maximal ideal of $W(k)[[T_1, T_2]]$ whose reduction modulo $(p, T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$ is non-zero. As $W(k)[[T_1, T_2]]/(p - h)$ is p-quasi-healthy (cf. the case $d = 2$), from Proposition 25 we get that R is quasi-healthy. This proves Theorem 3.
We prove Corollary 4. Thus $\dim R = d \geq 2$ and $p \notin \mathfrak{m}^p$. As in the previous paragraph we argue that we can assume that $R = \hat{R}$ is complete with algebraically closed residue class field k. We write $R = \mathfrak{S}/(p - h)$ where $h \in (T_1, \ldots, T_d)$ is such that its reduction $\bar{h} \in \bar{\mathfrak{S}} = \mathfrak{S}/p\mathfrak{S}$ modulo p is a power series of order $e = \operatorname{ord}(\bar{h}) \leq p - 1$. Due to Noether normalization theorem we can assume that $\bar{h}$ contains the monom T_1^e. We set $R' := \mathfrak{S}/(p - h, T_3, \ldots, T_d)$; if $d = 2$, then $R' = R$. From Proposition 25 applied to the epimorphism $R \twoheadrightarrow R'$, we get that it suffices to show that R' is quasi-healthy and p-quasi-healthy. Thus in order not to complicate the notations, we can assume that $d = 2$ (i.e., $R = R'$). As $e \leq p - 1$, the reduction of $\bar{h}$ modulo the ideal $(T_1^p, T_2^p, T_1^{p-1}T_2^{p-1})$ is non-zero. Thus Corollary 4 follows from Theorem 3. □

5.3 Example

Let R be a regular local of mixed characteristic $(0, p)$ such that the strict completion of R is isomorphic to

$$C_k[[T_1, \ldots, T_d]]/(p - T_1^{e_1} \cdot \ldots \cdot T_m^{e_m})$$

where C_k is a Cohen ring of the field k, where $1 \leq m \leq d$, and where the m-tuple $(e_1, \ldots, e_m) \in \mathbb{N}^m$ has the property that there exists a disjoint union $\{1, \ldots, m\} = I_1 \bigsqcup I_2$ for which we have $m_1 := \sum_{i \in I_1} e_i \in \{1, \ldots, p-1\}$ and $m_2 := \sum_{i \in I_2} e_i \in \{0, \ldots, p-2\}$.
To check that R is quasi-healthy we can assume that the field k is algebraically closed and that $R = W(k)[[T_1, \ldots, T_d]]/(p - T_1^{e_1} \cdot \ldots \cdot T_m^{e_m})$ (thus $C_k = W(k)$).

We consider the ring epimorphism $R \twoheadrightarrow R' := W(k)[[T_1, T_2]]/(p - T_1^{m_1} T_2^{m_2})$ that maps T_i with $i \in I_1$ to T_1, that maps T_i with $i \in I_2$ to T_2, and that maps T_i with $i > m$ to 0. From Theorem 3 we get that R is quasi-healthy.
Concrete example: if $1 \leq m \leq \min\{d, 2p-3\}$ and if the strict completion of R is $C_k[[T_1, \ldots, T_d]]/(p - T_1 \cdot \ldots \cdot T_m)$, then R is quasi-healthy. From this and Corollary 5 we get that each étale scheme over $\operatorname{Spec} O[T_1, \ldots, T_d]/(p - T_1 \cdot \ldots \cdot T_m)$ is healthy regular, provided O is a discrete valuation ring of mixed characteristic $(0, p)$ and index of ramification 1.

5.4 Regular schemes which are not (p-) healthy

Let R be a local regular ring of dimension 2 and mixed characteristic $(0, p)$. Let $\mathfrak{m}$ be the maximal ideal of R. Let $U = \operatorname{Spec} R \setminus \{\mathfrak{m}\}$.
The ring R is (p-) quasi-healthy if and only if $\operatorname{Spec} R$ is (p-) healthy regular. The next lemma provides an easy criterion for when R is not (p-) quasi-healthy.

Lemma 27 *We assume that there exists a homomorphism $H \to D$ of finite flat group schemes over* $\operatorname{Spec} R$ *which is not an epimorphism and whose restriction to U is an epimorphism. Then R is neither quasi-healthy nor p-quasi-healthy.*

Proof. We embed the Cartier dual D^{t} of D into an abelian scheme A over $\operatorname{Spec} R$, cf. [BBM], Theorem 3.1.1. The Cartier dual homomorphism $H_U^{\mathrm{t}} \to D_U^{\mathrm{t}}$ is a closed immersion. The abelian scheme A_U/H_U^{t} over U does not extend to an abelian scheme over $\operatorname{Spec} R$. Based on [R1], Chapter IX, Corollary 1.4, the argument for this is similar to the one used to prove that (d) implies (c) in Lemma 20. Thus R is not quasi-healthy. From Proposition 23 (a) we get that the p-divisible group of A_U/H_U^{t} does not extend to $\operatorname{Spec} R$. Thus the fact that R is not p-quasi-healthy follows from either Lemma 20 or Proposition 23 (a). □

Based on Lemma 27, the following theorem adds many examples to the classical example of Raynaud–Gabber.

Theorem 28 *We consider the ring $\mathfrak{S} = W(k)[[T_1, T_2]]$. Let $h \in (T_1, T_2) \setminus p\mathfrak{S}$. Let $R := \mathfrak{S}/(p - h)$. Let $\bar{\mathfrak{S}} := \mathfrak{S}/p\mathfrak{S}$ and let $\bar{h}$ be the reduction of h modulo p. We assume that one of the following three properties hold:*

(i) The element $\bar{h}$ is divisible by u^p, where u is a power series in the maximal ideal of $\bar{\mathfrak{S}}$ (the class of rings R for which (i) holds includes $O[[T]]$, where O is a totally ramified discrete valuation ring extension of $W(k)$ of index of ramification at least equal to p).

(ii) There exists a regular sequence u, v in $\bar{\mathfrak{S}}$ such that $u^{p-1} v^{p-1}$ divides $\bar{h}$.

(iii) We can write $\bar{h} = (aT_1^p + bT_2^p + cT_1^{p-1} T_2^{p-1})c$, where $a, b, c \in \bar{\mathfrak{S}}$.

Then R is neither p-quasi-healthy nor quasi-healthy.

Proof. It is enough to construct a homomorphism $\beta : H \to D$ of connected finite flat group schemes over $\operatorname{Spec} R$ which is not an epimorphism but whose restriction to U is an epimorphism, cf. Lemma 27.
We will construct H and D by specifying their Breuil modules (M, φ) and (N, τ) (respectively) associated to a standard frame for R. We first present with full details the case (i) and then we will only mention what are the changes required to be made for the other two cases (ii) and (iii).
We assume that the condition (i) holds. We set $M = \bar{\mathfrak{S}}^3$ and we identify $M^{(\sigma)}$ with $\bar{\mathfrak{S}}^3$. We choose an element $t \in \bar{\mathfrak{S}}$ such that t and u are a regular sequence in $\bar{\mathfrak{S}}$. We define the homomorphism φ by the following matrix:

$$\Gamma = \begin{pmatrix} 0 & 0 & u^p \\ t - t^p u^{p-1} & u & (u - t^{p-1})(t - t^p u^{p-1}) \\ u^{p-1} & 0 & u^{p-1}(u - t^{p-1}) \end{pmatrix}.$$

It is easy to see that there exists a matrix $\Delta \in M_{3\times 3}(\bar{\mathfrak{S}})$ such that

$$\Delta\Gamma = \Gamma\Delta = u^p I_3,$$

where I_3 is the unit matrix. It follows that the cokernel of φ is annihilated by u^p and thus also by $\bar{h}$. Moreover the image of φ is contained in $(t, u)M$. Therefore (M, φ) is the Breuil module H of a connected finite flat group scheme over $\operatorname{Spec} R$ annihilated by p.
We set $N = \bar{\mathfrak{S}}$ and $N^{(\sigma)} = \bar{\mathfrak{S}}$ and we define τ as the multiplication by u^p. This defines another connected finite flat group scheme D over $\operatorname{Spec} R$ annihilated by p.
One easily checks the following equation of matrices:

$$(t^p, u^p, (tu)^p)\Gamma = u^p(t, u, tu).$$

This equation shows that the $\mathfrak{S}$-linear map $M \to N$ defined by the matrix (t, u, tu) is a morphism of Breuil modules

$$\alpha : (M, \varphi) \to (N, \tau).$$

As α is not surjective, the homomorphism $\beta : H \to D$ associated to α is not an epimorphism. Let $\mathfrak{p} \neq \mathfrak{m}$ be a prime ideal of R which contains p. The base change of α by $\kappa_{\mathfrak{p}} : \mathfrak{S} \to W(\kappa(\mathfrak{p})^{\mathrm{perf}})$ (of Section 2) is an epimorphism as the cokernel of α is k. This implies that $\beta_U : H_U \to D_U$ is an epimorphism.
We assume that the condition (ii) holds. The proof in this case is similar to the case (i) but with the definitions of M, Γ, τ, and $M \to N$ modified as follows. Let $M = \bar{\mathfrak{S}}^2$. Let

$$\Gamma = \begin{pmatrix} u^{p-1} & 0 \\ 0 & v^{p-1} \end{pmatrix}.$$

Let τ be defined by $(uv)^{p-1}$. Let $M \to N$ be defined by the matrix $(v\ u)$.

We assume that the condition (iii) holds. Let $M = \bar{\mathfrak{S}}^2$. Let

$$\Gamma = \begin{pmatrix} aT_1 + cT_2^{p-1} & aT_2 \\ bT_1 & bT_2 + cT_1^{p-1} \end{pmatrix}.$$

Let τ be defined by $aT_1^p + bT_2^p + cT_1^{p-1}T_2^{p-1}$. Let $M \to N$ be defined by the matrix $(T_1\ T_2)$. The determinant of Γ is $\bar{h}$. □

6 Integral models and Néron models

Let O be a discrete valuation ring of mixed characteristic $(0, p)$ and of index of ramification at most $p-1$. Let K be the field of fractions of O. A flat O-scheme $\bigstar$ is said to have the *extension property*, if for each O-scheme X which is a healthy regular scheme, every morphism $X_K \to \bigstar_K$ of K-schemes extends uniquely to a morphism $X \to \bigstar$ of O-schemes (cf. [V1], Definition 3.2.3 3)).

Lemma 29 *Let Z_K be a regular scheme which is formally smooth over* $\operatorname{Spec} K$*. Then there exists at most one regular scheme which is a formally smooth O-scheme, which has the extension property, and whose fibre over* $\operatorname{Spec} K$ *is Z_K.*

Proof. Let Z_1 and Z_2 be two regular schemes which are formally smooth over $\operatorname{Spec} O$, which satisfy the identity $Z_{1,K} = Z_{2,K} = Z_K$, and which have the extension property. Both Z_1 and Z_2 are healthy regular schemes, cf. Corollary 5. Thus the identity $Z_{1,K} = Z_{2,K}$ extends naturally to morphisms $Z_1 \to Z_2$ and $Z_2 \to Z_1$, cf. the fact that both Z_1 and Z_2 have the extension property. Due to the uniqueness part of the extension property, the composite morphisms $Z_1 \to Z_2 \to Z_1$ and $Z_2 \to Z_1 \to Z_2$ are identity automorphisms. Thus the identity $Z_{1,K} = Z_{2,K}$ extends uniquely to an isomorphism $Z_1 \to Z_2$. □

Corollary 30 *The integral canonical models of Shimura varieties defined in [V1], Definition 3.2.3 6) are unique, provided they are over the spectrum of a discrete valuation ring O as above.*

Let $d \geq 1$ and $n \geq 3$ be natural numbers. We assume that n is prime to p. Let $\mathcal{A}_{d,1,n}$ be the Mumford moduli scheme over $\operatorname{Spec} \mathbb{Z}[\frac{1}{n}]$ that parameterizes principally polarized abelian scheme over $\operatorname{Spec} \mathbb{Z}[\frac{1}{n}]$-schemes which are of relative dimension d and which have level-n symplectic similitude structures (cf. [MFK], Theorems 7.9 and 7.10). For Néron models over Dedekind domains we refer to [BLR], Chapter I, Subsection 1.2, Definition 1.

Theorem 31 *Let $\mathcal{D}$ be a Dedekind domain which is a flat $\mathbb{Z}[\frac{1}{n}]$-algebra. Let $\mathcal{K}$ be the field of fractions of $\mathcal{D}$. We assume that the following two things hold:*

(i) the only local ring of $\mathcal{D}$ whose residue class field has characteristic 0*, is $\mathcal{K}$;*

(ii) if v is a prime of $\mathcal{D}$ whose residue class field has a prime characteristic $p_v \in \mathbb{N}^*$, then the index of ramification of the local ring of v is at most $p_v - 1$.

Let $\mathcal{N}$ be a finite $\mathcal{A}_{d,1,n,\mathcal{D}}$-scheme which is a projective, smooth $\mathcal{D}$-scheme. Then $\mathcal{N}$ is the Néron model over $\mathcal{D}$ of its generic fibre $\mathcal{N}_{\mathcal{K}}$.

Proof. Let Y be a smooth $\mathcal{D}$-scheme. Let $\delta_{\mathcal{K}} : Y_{\mathcal{K}} \to \mathcal{N}_{\mathcal{K}}$ be a morphism of $\mathcal{K}$-scheme. Let V be an open subscheme of Y which contains $Y_{\mathcal{K}}$ and all generic points of fibres of Y in positive characteristic and for which $\delta_{\mathcal{K}}$ extends uniquely to a morphism $\delta_V : V \to \mathcal{N}$ (cf. the projectiveness of $\mathcal{N}$). Let $(\mathcal{B}_V, \lambda_V)$ be the pull back to V of the universal principally polarized abelian scheme over $\mathcal{A}_{d,1,n,\mathcal{D}}$ via the composite morphism $\nu_V : V \to \mathcal{N} \to \mathcal{A}_{d,1,n,\mathcal{D}}$. From Corollary 5 we get that $\mathcal{B}_V$ extends uniquely to an abelian scheme $\mathcal{B}$ over Y. From [R1], Chapter IX, Corollary 1.4 we get that λ_V extends (uniquely) to a polarization λ of $\mathcal{B}$. The level-n symplectic similitude structure of $(\mathcal{B}_V, \lambda_V)$ defined naturally by ν_V extends uniquely to a level-n symplectic similitude structure of $(\mathcal{B}, \lambda)$, cf. the classical Nagata–Zariski purity theorem. Thus ν_V extends uniquely to a morphism $\nu : Y \to \mathcal{A}_{d,1,n,\mathcal{D}}$. As Y is a normal scheme, as $\mathcal{N}$ is finite over $\mathcal{A}_{d,1,n,\mathcal{D}}$, and as ν restricted to V factors through $\mathcal{N}$, the morphism ν factors uniquely through a morphism $\delta : Y \to \mathcal{N}$ which extends δ_V and thus also $\delta_{\mathcal{K}}$. Hence the Theorem follows from the very definition of Néron models. □

Remarks. (a) From Theorem 31 and [V3], Remark 4.4.2 and Example 4.5 we get that there exist plenty of Néron models over O whose generic fibres are not finite schemes over torsors of smooth schemes over $\mathrm{Spec}\, K$.
We can take $\mathcal{N}$ to be the pull back to O of those Néron models of Theorem 31 whose generic fibres have the above property (cf. [V3], Remark 4.5). If $p > 2$ and $e = p - 1$, then these Néron models $\mathcal{N}$ are new (i.e., their existence does not follow from [N], [BLR], [V1], [V2], or [V3]).
(b) One can use Theorem 28 (i) and Artin's approximation theorem to show that Theorem 31 does not hold in general if there exists a prime v of $\mathcal{D}$ whose residue class field has a prime characteristic $p_v \in \mathbb{N}^*$ and whose index of ramification is at least p_v. Counterexamples can be obtained using integral models of projective Shimura varieties of PEL type, cf. [V3], Corollary 4.3.

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Hankel Operators and the Dixmier Trace on Strictly Pseudoconvex Domains

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Abstract. Generalizing earlier results for the disc and the ball, we give a formula for the Dixmier trace of the product of $2n$ Hankel operators on Bergman spaces of strictly pseudoconvex domains in $\mathbf{C}^n$. The answer turns out to involve the dual Levi form evaluated on boundary derivatives of the symbols. Our main tool is the theory of generalized Toeplitz operators due to Boutet de Monvel and Guillemin.

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1. Introduction

Let Ω be a bounded strictly pseudoconvex domain in $\mathbf{C}^n$ with smooth boundary, and $L^2_{\text{hol}}(\Omega)$ the Bergman space of all holomorphic functions in $L^2(\Omega)$. For a bounded measurable function f on Ω, the Toeplitz and the Hankel operator with symbol f are the operators $\mathbf{T}_f : L^2_{\text{hol}}(\Omega) \to L^2_{\text{hol}}(\Omega)$ and $H_f : L^2_{\text{hol}}(\Omega) \to L^2(\Omega) \ominus L^2_{\text{hol}}(\Omega)$, respectively, defined by

$$\mathbf{T}_f g := \mathbf{\Pi}(fg), \quad H_f g := (I - \mathbf{\Pi})(fg), \tag{1}$$

where $\mathbf{\Pi} : L^2(\Omega) \to L^2_{\text{hol}}(\Omega)$ is the orthogonal projection. It has been known for some time that for f holomorphic and $n > 1$, the Hankel operator $H_{\overline{f}}$

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belongs to the Schatten ideal $\mathcal{S}^p$ if and only if f is in the diagonal Besov space $B^p(\Omega)$ and $p > 2n$, or f is constant (so $H_f = 0$) and $p \leq 2n$; see Arazy, Fisher and Peetre [1] for $\Omega = \mathbf{B}^n$, the unit ball of $\mathbf{C}^n$, and Li and Luecking [21] for general smoothly bounded strictly pseudoconvex domains Ω. This phenomenon is called a *cutoff* at $p = 2n$. In dimension $n = 1$, the situation is slightly different, in that the cutoff occurs not at $p = 2$ but at $p = 1$. One can rephrase the above results also in terms of membership in the Schatten classes of the commutators $[\mathbf{T}_{\overline{f}}, \mathbf{T}_g] := \mathbf{T}_{\overline{f}}\mathbf{T}_g - \mathbf{T}_g\mathbf{T}_{\overline{f}}$ of Toeplitz operators. In fact, it is immediate from (1) that

$$\mathbf{T}_{\overline{f}g} - \mathbf{T}_g\mathbf{T}_{\overline{f}} = H^*_{\overline{g}} H_{\overline{f}},$$

and also that $\mathbf{T}_{\overline{f}}\mathbf{T}_g = \mathbf{T}_{\overline{f}g}$ if f or g is holomorphic; thus for holomorphic f and g

$$[\mathbf{T}_{\overline{f}}, \mathbf{T}_g] = H^*_{\overline{g}} H_{\overline{f}}.$$

In any case, it follows that there are no nonzero trace-class Hankel operators $H_{\overline{f}}$, with f holomorphic, if $n = 1$, and similarly the product $H^*_{\overline{f}_1} H_{\overline{f}_2} \dots H^*_{\overline{f}_{2n-1}} H_{\overline{f}_{2n}} = [\mathbf{T}_{\overline{f}_2}, \mathbf{T}_{f_1}] \dots [\mathbf{T}_{\overline{f}_{2n}}, \mathbf{T}_{f_{2n-1}}]$, with $f_1, \dots, f_{2n}$ holomorphic, is never trace-class if $n > 1$. In particular, there is no hope for $n > 1$ of having an analogue of the well-known formula for the unit disc,

$$\text{tr}[\mathbf{T}_{\overline{f}}, \mathbf{T}_f] = \int_{\mathbf{D}} |f'(z)|^2 \, dm(z) \tag{2}$$

expressing the trace of the commutator $[\mathbf{T}_{\overline{f}}, \mathbf{T}_f]$ as the square of the Dirichlet norm of the holomorphic function f, which is one of the best known Moebius invariant integrals. (This formula actually holds for Toeplitz operators on any Bergman space of a bounded planar domain, if the Lebesgue area measure $dm(z)$ is replaced by an appropriate measure associated to the domain, see [2].) A remarkable substitute for (2) on the unit ball $\mathbf{B}^n$ is the result of Helton and Howe [19], who showed that for smooth functions $f_1, \dots, f_{2n}$ on the closed ball, the complete anti-symmetrization $[\mathbf{T}_{f_1}, \mathbf{T}_{f_2}, \dots, \mathbf{T}_{f_{2n}}]$ of the $2n$ operators $\mathbf{T}_{f_1}, \dots, \mathbf{T}_{f_{2n}}$ is trace-class and

$$\text{tr}[\mathbf{T}_{f_1}, \mathbf{T}_{f_2}, \dots, \mathbf{T}_{f_{2n}}] = \int_{\mathbf{B}^n} df_1 \wedge df_2 \wedge \dots \wedge df_{2n}.$$

There is, however, a generalization of (2) to the unit ball $\mathbf{B}^n$, $n > 1$, in a different direction — using the Dixmier trace. This may be notable especially in view of the prominent applications of the Dixmier trace in noncommutative differential geometry [9].

Namely, it was shown by the present authors and Guo [12] that for $f_1, \dots, f_n$ and $g_1, \dots, g_n$ smooth on the closed ball, the product $[\mathbf{T}_{f_1}, \mathbf{T}_{g_1}] \dots [\mathbf{T}_{f_n}, \mathbf{T}_{g_n}]$ belongs to the Dixmier class $\mathcal{S}^{\text{Dixm}}$ and has Dixmier trace equal to

$$\text{Tr}_\omega([\mathbf{T}_{f_1}, \mathbf{T}_{g_1}] \dots [\mathbf{T}_{f_n}, \mathbf{T}_{g_n}]) = \frac{1}{n!} \int_{\partial \mathbf{B}^n} \prod_{j=1}^n \{f_j, g_j\}_b \, d\sigma, \tag{3}$$

where $d\sigma$ is the normalized surface measure on $\partial\mathbf{B}^n$ and $\{f,g\}_b$ is the "boundary Poisson bracket" given by

$$\{f,g\}_b := \sum_{j=1}^n \Big(\frac{\partial f}{\partial \overline{z}_j}\frac{\partial g}{\partial z_j} - \frac{\partial f}{\partial z_j}\frac{\partial g}{\partial \overline{z}_j}\Big) - (\overline{R}fRg - Rf\overline{R}g),$$

with $\overline{R} := \sum_{j=1}^n \overline{z}_j \frac{\partial}{\partial \overline{z}_j}$ and $R := \sum_{j=1}^n z_j \frac{\partial}{\partial z_j}$ the anti-holomorphic and the holomorphic part of the radial derivative, respectively. In particular, for f holomorphic on $\mathbf{B}^n$ and smooth on the closed ball, $(H^*_{\overline{f}}H_{\overline{f}})^n = [\mathbf{T}_{\overline{f}}, \mathbf{T}_f]^n \in \mathcal{S}^{\mathrm{Dixm}}$ and

$$\mathrm{Tr}_\omega((H^*_{\overline{f}}H_{\overline{f}})^n) = \frac{1}{n!}\int_{\partial\mathbf{B}^n} \Big(\sum_{j=1}^n \Big|\frac{\partial f}{\partial z_j}\Big|^2 - |Rf|^2\Big)^n d\sigma.$$

Note that for $n=1$ the right-hand side vanishes, in accordance with the fact that in dimension 1 the cutoff occurs at $p=1$ instead of $p=2n=2$; in fact, it was shown by Rochberg and the first author [13] that for $n=1$ actually $|H_f| = (H^*_f H_f)^{1/2}$, rather than $H^*_f H_f$, is in the Dixmier class for any $f \in C^\infty(\overline{\mathbf{D}})$, and

$$\mathrm{Tr}_\omega(|H_f|) = \int_{\partial\mathbf{D}} |\overline{\partial} f|\, d\sigma,$$

so, in particular,

$$\mathrm{Tr}_\omega(|H_{\overline{f}}|) = \int_{\partial\mathbf{D}} |f'|\, d\sigma = \|f'\|_{H_1}$$

for $f \in C^\infty(\overline{\mathbf{D}})$ holomorphic on $\mathbf{D}$, where H^1 denotes the Hardy 1-space on the unit circle.

In this paper, we generalize the result of [12] to arbitrary bounded strictly pseudoconvex domains Ω with smooth boundary. Our result is that for any $2n$ functions $f_1, g_1, \dots, f_n, g_n \in C^\infty(\overline{\Omega})$,

$$\text{(4)} \quad \mathrm{Tr}_\omega(H^*_{f_1}H_{g_1}\dots H^*_{f_n}H_{g_n}) = \frac{1}{n!(2\pi)^n}\int_{\partial\Omega}\prod_{j=1}^n \mathcal{L}(\overline{\partial}_b g_j, \overline{\partial}_b f_j)\, \eta\wedge(d\eta)^{n-1},$$

where $\overline{\partial}_b$ stands for the boundary $\overline{\partial}$-operator [14], $\eta\wedge(d\eta)^{n-1}$ is a certain measure on $\partial\Omega$, and $\mathcal{L}$ stands for the dual of the Levi form on the anti-holomorphic tangent bundle; see §§ 2 and 4 below for the details.

In contrast to [12], where we were using the so-called pseudo-Toeplitz operators of Howe [18], our proof here relies on Boutet de Monvel's and Guillemin's theory of Toeplitz operators on the Hardy space $H^2(\partial\Omega)$ with pseudodifferential symbols. (This is also the approach used in [13], however the situation $\Omega = \mathbf{D}$ treated there is much more manageable.)

In fact, it turns out that for any classical pseudodifferential operator Q on $\partial\Omega$ of order $-n$, the corresponding Hardy-Toeplitz operator T_Q belongs to the Dixmier class and

$$\text{(5)} \qquad \operatorname{Tr}_\omega(T_Q) = \frac{1}{n!(2\pi)^n} \int_{\partial\Omega} \sigma_{-n}(Q)(x, \eta(x))\, \eta(x) \wedge (d\eta(x))^{n-1},$$

where $\sigma_{-n}(Q)$ is the principal symbol of Q, and η is a certain 1-form on $\partial\Omega$; see again §2 below for the details. In particular, in view of the results of Guillemin [16] [17], this means that on Toeplitz operators T_Q of order $\leq -n$, the Dixmier trace $\operatorname{Tr}_\omega T_Q$ coincides with the residual trace $\operatorname{Tr}_{\text{Res}} T_Q$, a quantity constructed using the meromorphic continuation of the ζ function of T_Q (Wodzicki [24], Boutet de Monvel [7], Ponge [23], Lesch [20], Connes [9]).

We recall the necessary prerequisites on the Dixmier trace, Hankel operators and the Boutet de Monvel-Guillemin theory in Section 2. The proofs of (5) and (4) appear in Sections 3 and 4, respectively. Some concluding comments are assembled in the final Section 5.

Throughout the paper, we will denote Bergman-space Toeplitz operators by $\mathbf{T}_f$, in order to distinguish them from the Hardy-space Toeplitz operators T_f and T_Q. Since Hankel operators on the Hardy space never appear in this paper, Hankel operators on the Bergman space are denoted simply by H_f.

2. Background

2.1 Generalized Toeplitz operators. Let r be a defining function for Ω, that is, $r \in C^\infty(\overline{\Omega})$, $r < 0$ on Ω, and $r = 0$, $\|\partial r\| > 0$ on $\partial\Omega$. Denote by η the restriction to $\partial\Omega$ of the 1-form $\operatorname{Im}(\partial r) = (\partial r - \overline{\partial} r)/2i$. The strict pseudoconvexity of Ω guarantees that η is a contact form, i.e. the half-line bundle

$$\Sigma := \{(x, \xi) \in \mathcal{T}^*(\partial\Omega) : \ \xi = t\eta_x, \ t > 0\}$$

is a symplectic submanifold of $\mathcal{T}^*(\partial\Omega)$. Equip $\partial\Omega$ with a measure with smooth positive density, and let $L^2(\partial\Omega)$ be the Lebesgue space with respect to this measure. The Hardy space $H^2(\partial\Omega)$ is the subspace in $L^2(\partial\Omega)$ of functions whose Poisson extension is holomorphic in Ω; or, equivalently, the closure in $L^2(\partial\Omega)$ of $C^\infty_{\text{hol}}(\partial\Omega)$, the space of boundary values of all the functions in $C^\infty(\overline{\Omega})$ that are holomorphic on Ω. (In dimensions greater than 1, $H^2(\partial\Omega)$ can also be characterized as the null-space of the $\overline{\partial}_b$-operator, which will appear in Section 4 further on.) We will also denote by $W^s(\partial\Omega)$, $s \in \mathbf{R}$, the Sobolev spaces on $\partial\Omega$, and by $W^s_{\text{hol}}(\partial\Omega)$ the corresponding subspaces of nontangential boundary values of functions holomorphic in Ω. (Thus $W^0(\partial\Omega) = L^2(\partial\Omega)$ and $W^0_{\text{hol}}(\partial\Omega) = H^2(\partial\Omega)$.)

Unless otherwise specified, by a pseudodifferential operator or Fourier integral operator (ΨDO or FIO for short) on $\partial\Omega$ we will always mean an operator which is "classical", i.e. whose total symbol (or amplitude) in any local coordinate system has an asymptotic expansion

$$p(x,\xi) \sim \sum_{j=0}^{\infty} p_{m-j}(x,\xi),$$

where p_{m-j} is C^∞ in x, ξ, and is positive homogeneous of degree $m-j$ in ξ for $|\xi| > 1$. Here j runs through nonnegative integers, while m can be any integer; and the symbol "$\sim$" means that the difference between p and $\sum_{j=0}^{k-1} p_{m-j}$ should belong to the Hörmander class S^{m-k}, for each $k = 0, 1, 2, \dots$. The set of all classical ΨDOs on $\partial\Omega$ as above (i.e. of order m) will be denoted by $\Psi^m_{\rm cl}$; and we set, as usual, $\Psi_{\rm cl} := \bigcup_{m\in\mathbf{Z}} \Psi^m_{\rm cl}$ and $\Psi^{-\infty} := \bigcap_{m\in\mathbf{Z}} \Psi^m_{\rm cl}$. The operators in $\Psi^{-\infty}$ are precisely the *smoothing* operators, i.e. those given by a C^∞ Schwartz kernel; and for any $P, Q \in \Psi_{\rm cl}$, we will write $P \sim Q$ if $P - Q$ is smoothing. Note that if $P \in \Psi^m_{\rm cl}$, then P is continuous from $W^s(\partial\Omega)$ into $W^{s-m}(\partial\Omega)$, for any $s \in \mathbf{R}$.

For $Q \in \Psi^m_{\rm cl}$, the *generalized Toeplitz operator* $T_Q : W^m_{\rm hol}(\partial\Omega) \to H^2(\partial\Omega)$ is defined as

$$T_Q = \Pi Q,$$

where $\Pi : L^2(\partial\Omega) \to H^2(\partial\Omega)$ is the orthogonal projection (the Szegö projection). Alternatively, one may view T_Q as the operator

$$T_Q = \Pi Q \Pi$$

on all of $W^m(\partial\Omega)$. Actually, T_Q maps continuously $W^s(\partial\Omega)$ into $W^{s-m}_{\rm hol}(\partial\Omega)$, for each $s \in \mathbf{R}$, because Π is bounded on $W^s(\partial\Omega)$ for any $s \in \mathbf{R}$ (see [6]).

It is known that the generalized Toeplitz operators T_P, $P \in \Psi_{\rm cl}$, have the following properties.

(P1) They form an algebra which is, modulo smoothing operators, locally isomorphic to the algebra of classical ΨDOs on $\mathbf{R}^n$.

(P2) In fact, for any T_Q there exists a ΨDO P of the same order such that $T_Q = T_P$ and $P\Pi = \Pi P$.

(P3) If P, Q are of the same order and $T_P = T_Q$, then the principal symbols $\sigma(P)$ and $\sigma(Q)$ coincide on Σ. One can thus define unambiguously the *order* of a generalized Toeplitz operator as $\mathrm{ord}(T_Q) := \min\{\mathrm{ord}(P) : T_P = T_Q\}$, and its *principal symbol* (or just "symbol") as $\sigma(T_Q) := \sigma(Q)|_\Sigma$ if $\mathrm{ord}(Q) = \mathrm{ord}(T_Q)$. (The symbol is undefined if $\mathrm{ord}(T_Q) = -\infty$.)

(P4) The order and the symbol are multiplicative: $\mathrm{ord}(T_P T_Q) = \mathrm{ord}(T_P) + \mathrm{ord}(T_Q)$ and $\sigma(T_P T_Q) = \sigma(T_P)\sigma(T_Q)$.

(P5) If $\mathrm{ord}(T_Q) \le 0$, then T_Q is a bounded operator on $L^2(\partial\Omega)$; if $\mathrm{ord}(T_Q) < 0$, then it is even compact.

(P6) If $Q \in \Psi^m_{\rm cl}$ and $\sigma(T_Q) = 0$, then there exists $P \in \Psi^{m-1}_{\rm cl}$ with $T_P = T_Q$. In particular, if $T_Q \sim 0$, then there exists a ΨDO $P \sim 0$ such that $T_Q = T_P$.

(P7) We will say that a generalized Toeplitz operator T_Q of order m is *elliptic* if $\sigma(T_Q)$ does not vanish. Then T_Q has a parametrix, i.e. there exists a Toeplitz operator T_P of order $-m$, with $\sigma(T_P) = \sigma(T_Q)^{-1}$, such that $T_Q T_P \sim I_{H^2(\partial\Omega)} \sim T_P T_Q$.

We refer to the book [5], especially its Appendix, and to the paper [4] (which we have loosely followed in this section) for the proofs and additional information on generalized Toeplitz operators.

2.2 The Poisson operator. Let $\mathbf{K}$ denote the Poisson extension operator on Ω, i.e. $\mathbf{K}$ solves the Dirichlet problem

$$\Delta \mathbf{K} u = 0 \quad \text{on } \Omega, \qquad \mathbf{K} u|_{\partial\Omega} = u. \tag{6}$$

(Thus $\mathbf{K}$ acts from functions on $\partial\Omega$ into functions on Ω. Here Δ is the ordinary Laplace operator.) By the standard elliptic regularity theory (see e.g. [22]), $\mathbf{K}$ acts continuously from $W^s(\partial\Omega)$ onto the subspace $W^{s+1/2}_{\text{harm}}(\Omega)$ of all harmonic functions in $W^{s+1/2}(\Omega)$. In particular, it is continuous from $L^2(\partial\Omega)$ into $L^2(\Omega)$, and thus has a continuous Hilbert space adjoint $\mathbf{K}^* : L^2(\Omega) \to L^2(\partial\Omega)$. The composition

$$\mathbf{K}^*\mathbf{K} =: \Lambda$$

is known to be an elliptic positive ΨDO on $\partial\Omega$ of order -1. We have

$$\Lambda^{-1}\mathbf{K}^*\mathbf{K} = I_{L^2(\partial\Omega)}, \tag{7}$$

while

$$\mathbf{K}\Lambda^{-1}\mathbf{K}^* = \mathbf{\Pi}_{\text{harm}},$$

the orthogonal projection in $L^2(\Omega)$ onto the subspace $L^2_{\text{harm}}(\Omega)$ of all harmonic functions. (Indeed, from (7) it is immediate that the left-hand side acts as the identity on the range of $\mathbf{K}$, while it trivially vanishes on $\operatorname{Ker}\mathbf{K}^* = (\operatorname{Ran}\mathbf{K})^\perp$.) Comparing (7) with (6), we also see that the restriction

$$\gamma := \Lambda^{-1}\mathbf{K}^*|_{L^2_{\text{harm}}(\Omega)}$$

is the operator of "taking the boundary values" of a harmonic function. Again, by elliptic regularity, γ extends to a continuous operator from $W^s_{\text{harm}}(\Omega)$ onto $W^{s-1/2}(\partial\Omega)$, for any $s \in \mathbf{R}$, which is the inverse of $\mathbf{K}$.

The operators

$$\Lambda_w := \mathbf{K}^* w \mathbf{K},$$

with w a smooth function on $\overline{\Omega}$, are governed by a calculus developed by Boutet de Monvel [3]. It was shown there that for w of the form

$$w = r^m g, \qquad m = 0, 1, 2, \dots,\ g \in C^\infty(\overline{\Omega}), \tag{8}$$

Λ_w is a ΨDO on $\partial\Omega$ of order $-m-1$, with symbol

$$\sigma(\Lambda_w)(x,\xi) = \frac{(-1)^m m!}{2|\xi|^{m+1}}\, g(x)\, \|\eta_x\|^m. \tag{9}$$

(In particular, $\sigma(\Lambda)(x,\xi) = 1/2|\xi|$.)
By abstract Hilbert space theory, $\mathbf{K}$ has, as an operator from $L^2(\partial\Omega)$ into $L^2(\Omega)$, the polar decomposition

$$\mathbf{K} = U(\mathbf{K}^*\mathbf{K})^{1/2} = U\Lambda^{1/2}, \tag{10}$$

where U is a partial isometry with initial space $\overline{\operatorname{Ran}\mathbf{K}^*} = (\operatorname{Ker}\mathbf{K})^\perp$ and final space $\overline{\operatorname{Ran}\mathbf{K}}$; that is, U is a unitary operator from $L^2(\partial\Omega)$ onto $L^2_{\text{harm}}(\Omega)$.
The operators γ, $\mathbf{K}$ and $U = \mathbf{K}\Lambda^{-1/2}$ can be used to "transfer" operators on $L^2_{\text{harm}}(\Omega) \subset L^2(\Omega)$ into operators on $L^2(\partial\Omega)$. The following proposition appears as Proposition 8 in [11]; we reproduce its (short) proof here for completeness.

Proposition 1. $\gamma\mathbf{\Pi}\mathbf{K} = T_\Lambda^{-1}\Pi\Lambda$.

Proof. Set $\mathbf{\Pi}_\Lambda := \mathbf{K}T_\Lambda^{-1}\Pi\Lambda\gamma$, an operator on $L^2_{\text{harm}}(\Omega)$; we need to show that $\mathbf{\Pi}_\Lambda = \mathbf{\Pi}|_{L^2_{\text{harm}}}$. Since $T_\Lambda^{-1}\Pi\Lambda$ acts as the identity on the range of Π, it is immediate that $\mathbf{\Pi}_\Lambda^2 = \mathbf{\Pi}_\Lambda$; furthermore, $\mathbf{\Pi}_\Lambda = \mathbf{K}T_\Lambda^{-1}\Pi\mathbf{K}^* = \mathbf{K}\Pi T_\Lambda^{-1}\Pi\mathbf{K}^*$ is evidently self-adjoint. Thus $\mathbf{\Pi}_\Lambda$ is the orthogonal projection in $L^2_{\text{harm}}(\Omega)$ onto $\operatorname{Ran}\mathbf{\Pi}_\Lambda$. But

$$\begin{aligned}\operatorname{Ran}\mathbf{\Pi}_\Lambda &= (\operatorname{Ker}\mathbf{\Pi}_\Lambda)^\perp = (\operatorname{Ker}\mathbf{K}\Pi T_\Lambda^{-1}\Pi\mathbf{K}^*)^\perp = (\operatorname{Ker}T_\Lambda^{-1/2}\Pi\mathbf{K}^*)^\perp \\ &= (\operatorname{Ker}\Pi\mathbf{K}^*)^\perp = \overline{\operatorname{Ran}\mathbf{K}\Pi} = \overline{\mathbf{K}H^2(\partial\Omega)} \\ &= \overline{W^{1/2}_{\text{hol}}(\Omega)} = L^2_{\text{hol}}(\Omega).\end{aligned}$$

So, indeed, $\mathbf{\Pi}_\Lambda = \mathbf{\Pi}$. □

Similarly to (10), the bounded (in fact — since Λ is of order < 0 — even compact) operator $\Lambda^{1/2}\Pi$ on $L^2(\partial\Omega)$ has polar decomposition

$$\Lambda^{1/2}\Pi = W(\Pi\Lambda\Pi)^{1/2} = WT_\Lambda^{1/2},$$

where W is a partial isometry with initial space $\overline{\operatorname{Ran}\Pi\Lambda^{1/2}} = H^2(\partial\Omega)$ and final space $\overline{\operatorname{Ran}\Lambda^{1/2}\Pi} = \overline{\Lambda^{1/2}H^2(\partial\Omega)}$; in particular,

$$W^*W = I \quad \text{on } H^2(\partial\Omega). \tag{11}$$

The following proposition is analogous to Corollary 9 of [11].

Proposition 2. *Let $w \in C^\infty(\overline{\Omega})$ be of the form* (8). *Then*

$$U^* \mathbf{T}_w U = W T_\Lambda^{-1/2} T_{\Lambda_w} T_\Lambda^{-1/2} W^* = W T_{Q_w} W^*,$$

where Q_w is a ΨDO on $\partial\Omega$ of order $-m$ with

$$\sigma(Q_w)(x,\xi)|_\Sigma = \frac{(-1)^m m!}{|\xi|^m} g(x) \, \|\eta_x\|^m.$$

Proof. By Proposition 1, $\mathbf{\Pi K} = \mathbf{K} T_\Lambda^{-1} \Pi \Lambda = \mathbf{K} \Pi T_\Lambda^{-1} \Pi \Lambda$; hence

$$\begin{aligned} U^* \mathbf{T}_w U &= \Lambda^{-1/2} \mathbf{K}^* \mathbf{\Pi} w \mathbf{\Pi K} \Lambda^{-1/2} \\ &= \Lambda^{1/2} \Pi T_\Lambda^{-1} \Pi \mathbf{K}^* w \mathbf{K} \Pi T_\Lambda^{-1} \Pi \Lambda^{1/2} \\ &= \Lambda^{1/2} \Pi T_\Lambda^{-1} \Pi \Lambda_w \Pi T_\Lambda^{-1} \Pi \Lambda^{1/2} \\ &= \Lambda^{1/2} \Pi T_\Lambda^{-1} T_{\Lambda_w} T_\Lambda^{-1} \Pi \Lambda^{1/2} \\ &= W T_\Lambda^{-1/2} T_{\Lambda_w} T_\Lambda^{-1/2} W^*, \end{aligned}$$

proving the first equality. The second equality follows from (9) and the properties (P1) and (P4). $\square$

2.3 The Dixmier trace. Recall that if A is a compact operator acting on a Hilbert space then its sequence of singular values $\{s_j(A)\}_{j=1}^\infty$ is the sequence of eigenvalues of $|A| = (A^*A)^{1/2}$ arranged in nonincreasing order. In particular if $A \gg 0$ this will also be the sequence of eigenvalues of A in nonincreasing order. For $0 < p < \infty$ we say that A is in the Schatten ideal $\mathcal{S}_p$ if $\{s_j(A)\} \in l^p(\mathbf{Z}_{>0})$. If $A \gg 0$ is in $\mathcal{S}_1$, the trace class, then A has a finite trace and, in fact, $\operatorname{tr}(A) = \sum_j s_j(A)$. If however we only know that

$$\begin{aligned} &s_j(A) = O(j^{-1}) \text{ or that} \\ &S_k(A) := \sum_{j=1}^k s_j(A) = O(\log(1+k)) \end{aligned}$$

then A may have infinite trace. However in this case we may still try to compute its *Dixmier trace*, $\operatorname{Tr}_\omega(A)$. Informally $\operatorname{Tr}_\omega(A) = \lim_k \frac{1}{\log k} S_k(A)$ and this will actually be true in the cases of interest to us. We begin with the definition. Select a continuous positive linear functional ω on $l^\infty(\mathbf{Z}_{>0})$ and denote its value on $a = (a_1, a_2, \ldots)$ by $\operatorname{Lim}_\omega(a_k)$. We require of this choice that $\operatorname{Lim}_\omega(a_k) = \lim a_k$ if the latter exists. We require further that ω be *scale invariant*; a technical requirement that is fundamental for the theory but will not be of further concern to us.

Let $\mathcal{S}^{\text{Dixm}}$ be the class of all compact operators A which satisfy

$$\Big(\frac{S_k(A)}{\log(1+k)}\Big) \in l^\infty. \tag{12}$$

With the norm defined as the l^∞-norm of the left-hand side of (12), $\mathcal{S}^{\mathrm{Dixm}}$ becomes a Banach space [15]. For a positive operator $A \in \mathcal{S}^{\mathrm{Dixm}}$, we define the Dixmier trace of A, $\mathrm{Tr}_\omega(A)$, as $\mathrm{Tr}_\omega(A) = \mathrm{Lim}_\omega(\frac{S_k(A)}{\log(1+k)})$. $\mathrm{Tr}_\omega(\cdot)$ is then extended by linearity to all of $\mathcal{S}^{\mathrm{Dixm}}$. Although this definition does depend on ω the operators A we consider are *measurable*, that is, the value of $\mathrm{Tr}_\omega(A)$ is independent of the particular choice of ω. We refer to [9] for details and for discussion of the role of these functionals.

It is a result of Connes [8] that if Q is a ΨDO on a compact manifold M of real dimension n and $\mathrm{ord}(Q) = -n$, then $Q \in \mathcal{S}^{\mathrm{Dixm}}$ and

$$\mathrm{Tr}_\omega(Q) = \frac{1}{n!(2\pi)^n} \int_{(\mathcal{T}^*M)_1} \sigma(Q). \tag{13}$$

(Here $(\mathcal{T}^*M)_1$ denotes the unit sphere bundle in the cotangent bundle $\mathcal{T}^*M$, and the integral is taken with respect to a measure induced by any Riemannian metric on M; since $\sigma(Q)$ is homogeneous of degree $-n$, the value of the integral is independent of the choice of such metric.) In the next section, we will see that for Toeplitz operators T_Q on $\partial\Omega$, $\Omega \subset \mathbf{C}^n$, the "right" order for T_Q to belong to $\mathcal{S}^{\mathrm{Dixm}}$ is not $-\dim_{\mathbf{R}} \partial\Omega = -(2n-1)$, but $-\dim_{\mathbf{C}} \Omega = -n$.

3. Dixmier trace of generalized Toeplitz operators

Let T be a positive self-adjoint generalized Toeplitz operator on $\partial\Omega$ of order 1 with $\sigma(T) > 0$. Let $0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \dots$ be the points of its spectrum (counting multiplicities) and let $N(\lambda)$ denote the number of λ_j's less than λ. It was shown in Theorem 13.1 in [5] that as $\lambda \to +\infty$,

$$N(\lambda) = \frac{\mathrm{vol}(\Sigma_T)}{(2\pi)^n}\lambda^n + O(\lambda^{n-1}), \tag{14}$$

where Σ_T is the subset of Σ where $\sigma(T) \le 1$, and $\mathrm{vol}(\Sigma_T)$ is its symplectic volume.

Using properties of generalized Toeplitz operators, it is easy to derive from here the formula for the Dixmier trace.

Theorem 3. *Let T be a generalized Toeplitz operator on $H^2(\partial\Omega)$ of order $-n$. Then $T \in \mathcal{S}^{\mathrm{Dixm}}$, and*

$$\mathrm{Tr}_\omega(T) = \frac{1}{n!(2\pi)^n} \int_{\partial\Omega} \sigma(T)(x,\eta_x)\, \eta \wedge (d\eta)^{n-1}.$$

In particular, T is measurable.

Proof. As the Dixmier trace is defined first on positive operators and then extended to all of $\mathcal{S}^{\mathrm{Dixm}}$ by linearity, while T may be split into its real and imaginary parts each of which can be expressed as a difference of two positive generalized Toeplitz operators of the same order, it is enough to prove the assertion when T is positive self-adjoint with $\sigma(T) > 0$. Then T is elliptic, and it follows from Seeley's theorem on complex powers of ΨDO's and from the property (P2) that $T^{-1/n}$ is also a generalized Toeplitz operator, with symbol $\sigma(T)^{-1/n}$ and of order 1 (see [10], Proposition 16, for the detailed argument). Thus the eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots$ of $T^{-1/n}$ satisfy (14). Consequently,

$$\begin{aligned} S_k(T) = \sum_{j=1}^{k} s_j(T) = \sum_{j=1}^{k} \lambda_j^{-n} &= \int_{[\lambda_1,\lambda_k]} \lambda^{-n}\, dN(\lambda) \\ &= \int_{[\lambda_1,\lambda_k]} \Big(\frac{c}{N(\lambda)} + O\big(N(\lambda)^{-1-\frac{1}{n}}\big) \Big)\, dN(\lambda) \\ &= \int_1^k \Big(\frac{c}{N} + O(N^{-1-\frac{1}{n}}) \Big)\, dN \\ &= c \log k + O(1). \end{aligned}$$

Here we have temporarily denoted $c := (2\pi)^{-n}\operatorname{vol}(\Sigma_{T^{-1/n}})$. Dividing by $\log(k+1)$ and letting k tend to infinity, it follows that $T \in \mathcal{S}^{\mathrm{Dixm}}$ and

$$\operatorname{Tr}_\omega(T) = \lim_{k\to\infty} \frac{S_k(T)}{\log(k+1)} = c. \tag{15}$$

Let us parameterize Σ as $(x, t\eta_x)$ with $x \in \partial\Omega$, $t > 0$. The subset $\Sigma_{T^{-1/n}}$ is then characterized by

$$\sigma(T)(x, t\eta_x)^{-1/n} \leq 1, \quad \text{or} \quad t \leq \sigma(T)(x,\eta_x)^{1/n}.$$

A routine computation, which we postpone to the next lemma, shows that the symplectic volume on Σ with respect to the above parameterization is given by $\frac{t^{n-1}}{(n-1)!}\, dt \wedge \eta(x) \wedge (d\eta(x))^{n-1}$. Consequently,

$$\begin{aligned} \operatorname{vol}(\Sigma_{T^{-1/n}}) &= \int_{\partial\Omega} \int_0^{\sigma(T)(x,\eta_x)^{1/n}} \frac{t^{n-1}}{(n-1)!}\, dt \wedge \eta \wedge (d\eta)^{n-1} \\ &= \frac{1}{n!} \int_{\partial\Omega} \sigma(T)(x,\eta_x)\, \eta \wedge (d\eta)^{n-1}. \end{aligned}$$

Combining this with (15) and the definition of c, the assertion follows. □

Remark 4. Observe that, in analogy with (13), the last integral is independent of the choice of the defining function. Indeed, if r is replaced by gr, with $g > 0$ on $\partial\Omega$, then $\eta = \operatorname{Im}(\partial r)$ is replaced by $g\eta$ (since $\partial(gr) = g\partial r$ on the set where $r = 0$), and $\eta \wedge (d\eta)^{n-1}$ by $g\eta \wedge (g\, d\eta + dg \wedge \eta)^{n-1} = g^n\, \eta \wedge (d\eta)^{n-1}$ (because $\eta \wedge \eta = 0$); as $\sigma(T)(x,\xi)$ is homogeneous of degree $-n$ in ξ, the integrand remains unchanged. □

Lemma 5. *With respect to the parameterization* $\Sigma = \{(x, t\eta_x) : x \in \partial\Omega, t > 0\}$, *the symplectic form on* Σ *is given by*

$$\omega = t\, d\eta + dt \wedge \eta = d(t\eta).$$

Consequently, the symplectic volume in the (x,t) *coordinates is given by*

$$\frac{\omega^n}{n!} = \frac{t^{n-1}}{(n-1)!}\, dt \wedge \eta \wedge (d\eta)^{n-1}.$$

We are supplying a proof of this simple fact below, since we were unable to locate it in the literature (though we expect that it must be at least implicitly contained e.g. somewhere in [5]).

Proof. Recall that if $(x_1, x_2, \dots, x_{2n-1})$ is a real coordinate chart on $\partial\Omega$ and (x,ξ) the corresponding local coordinates for a point $(x; \xi_1 dx_1 + \dots + \xi_{2n-1} dx_{2n-1})$ in $\mathcal{T}^*\partial\Omega$, then the form $\alpha = \xi_1 dx_1 + \dots + \xi_{2n-1} dx_{2n-1}$ is globally defined and the symplectic form is given by $\omega = d\alpha = d\xi_1 \wedge dx_1 + \dots + d\xi_{2n-1} \wedge dx_{2n-1}$. Since exterior differentiation commutes with restriction (or, more precisely, with the pullback j^* under the inclusion map $j : \Sigma \to \mathcal{T}^*\partial\Omega$), it follows that the symplectic form $\omega_\Sigma = j^*\omega$ on Σ is given by $\omega_\Sigma = d(j^*\alpha)$. As in our case $j^*\alpha = t\eta$, the first formula follows. (We will drop the subscript Σ from now on.) The second formula is immediate from the first since $\eta \wedge \eta = 0$ and $(d\eta)^n = 0$. □

The following corollary is immediate upon combining Theorem 3 and Proposition 2.

Corollary 6. *Assume that* $f \in C^\infty(\overline{\Omega})$ *vanishes at* $\partial\Omega$ *to order* n. *Then* $\mathbf{T}_f$ *belongs to the Dixmier class, is measurable, and*

$$\operatorname{Tr}_\omega(\mathbf{T}_f) = \frac{1}{n!(4\pi)^n} \int_{\partial\Omega} \mathfrak{N}^n f \, \frac{\eta \wedge (d\eta)^{n-1}}{\|\eta\|^n},$$

where $\mathfrak{N}$ *denotes the interior unit normal derivative.*

4. Dixmier trace for products of Hankel operators

It is known [5] that the symbol of the commutator of two generalized Toeplitz operators is given by the Poisson bracket (with respect to the symplectic structure of Σ) of their symbols:

$$\sigma([T_P, T_Q]) = \tfrac{1}{i}\{\sigma(T_P), \sigma(T_Q)\}_\Sigma.$$

We need an analogous formula for the semi-commutator $T_{PQ} - T_P T_Q$ of two generalized Toeplitz operators. Not surprisingly, it turns out to be given (at least in the cases of interest to us) by an appropriate "half" of the Poisson bracket.

Let us denote by $\mathcal{T}'' \subset \mathcal{T}\partial\Omega \otimes \mathbf{C}$ the anti-holomorphic complex tangent space to $\partial\Omega$, i.e. the elements of $\mathcal{T}''_x$, $x \in \partial\Omega$, are the vectors $\sum_{j=1}^n a_j \frac{\partial}{\partial \overline{z}_j}$, $a_j \in \mathbf{C}$, such that $\sum_j a_j \frac{\partial r}{\partial \overline{z}_j}(x) = 0$. (This notation follows [6], p. 141.) On the open subset $\mathcal{U}_m$ of $\partial\Omega$ where $\frac{\partial r}{\partial \overline{z}_m} \neq 0$ (as m ranges from 1 to n, these subsets cover all of $\partial\Omega$), $\mathcal{T}''$ is spanned by the $n-1$ vector fields

$$\overline{R}_j := \frac{\partial}{\partial \overline{z}_j} - \frac{\partial r/\partial \overline{z}_j}{\partial r/\partial \overline{z}_m} \frac{\partial}{\partial \overline{z}_m}, \qquad j \neq m.$$

(Thus $\overline{R}_j$ depends also on m, although this is not reflected by the notation.) The (similarly defined) holomorphic complex tangent space $\mathcal{T}'$ is, analogously, spanned on $\mathcal{U}_m$ by the $n-1$ vector fields

$$R_j := \frac{\partial}{\partial z_j} - \frac{\partial r/\partial z_j}{\partial r/\partial z_m} \frac{\partial}{\partial z_m}, \qquad j \neq m,$$

while the whole complex tangent space $\mathcal{T}\partial\Omega \otimes \mathbf{C}$ is spanned there by the R_j, $\overline{R}_j$ and

$$E := \sum_{j=1}^n \frac{\partial r}{\partial z_j} \frac{\partial}{\partial \overline{z}_j} - \frac{\partial r}{\partial \overline{z}_j} \frac{\partial}{\partial z_j}$$

(the "complex normal" direction).
The boundary d-bar operator $\overline{\partial}_b : C^\infty(\partial\Omega) \to C^\infty(\partial\Omega, \mathcal{T}''^*)$ is defined as the restriction

$$\overline{\partial}_b f := df|_{\mathcal{T}''},$$

or, more precisely, $\overline{\partial}_b f = d\tilde{f}|_{\mathcal{T}''}$ for any smooth extension $\tilde{f}$ of f to a neighbourhood of $\partial\Omega$ in $\mathbf{C}^n$ (the right-hand side is independent of the choice of such extension). On $\mathcal{U}_m$, $\mathcal{T}''^*$ admits $d\overline{z}_j|_{\mathcal{T}''}$, $j \neq m$, as a basis and

$$\overline{\partial}_b f = \sum_j \overline{R}_j f \, d\overline{z}_j|_{\mathcal{T}''}.$$

Under our parameterization of Σ by $(x,t) \in \partial\Omega \times \mathbf{R}_+$, the tangent bundle $\mathcal{T}\Sigma$ is identified with $\mathcal{T}\partial\Omega \times \mathbf{R}$, being spanned at each $(x, t\eta_x) \in \Sigma$ by $\overline{R}_j$, R_j, E and the extra vector $T := \frac{\partial}{\partial t}$. Recall that the Levi form L' is the Hermitian form on $\mathcal{T}'$ defined by

$$L'(X,Y) := \sum_{j,k=1}^n \frac{\partial^2 r}{\partial z_j \partial \overline{z}_k} X_j \overline{Y}_k \qquad \text{if } X = \sum_j X_j \frac{\partial}{\partial z_j},\ Y = \sum_k Y_k \frac{\partial}{\partial z_k}.$$

The strong pseudoconvexity of Ω means that L' is positive definite. Similarly, one has the positive-definite Levi form L'' on $\mathcal{T}''$ defined by

$$L''(X,Y) := \sum_{j,k=1}^n \frac{\partial^2 r}{\partial z_k \partial \overline{z}_j} X_j \overline{Y}_k \qquad \text{if } X = \sum_j X_j \frac{\partial}{\partial \overline{z}_j},\ Y = \sum_k Y_k \frac{\partial}{\partial \overline{z}_k}.$$

In terms of the complex conjugation $X \mapsto \overline{X}$ given by $\overline{X_j \frac{\partial}{\partial z_j}} = \overline{X}_j \frac{\partial}{\partial \overline{z}_j}$, mapping $\mathcal{T}'$ onto $\mathcal{T}''$ and vice versa, the two forms are related by

$$L''(X,Y) = L'(\overline{Y}, \overline{X}) \qquad \forall X, Y \in \mathcal{T}''. \tag{16}$$

By the usual formalism, L'' induces a positive definite Hermitian form[1] on the dual space $\mathcal{T}''^*$ of $\mathcal{T}''$; we denote it by $\mathcal{L}$. Namely, if L'' is given by a matrix $\mathbb{L}$ with respect to some basis $\{e_j\}$, then $\mathcal{L}$ is given by the inverse matrix $\mathbb{L}^{-1}$ with respect to the dual basis $\{\hat{e}_k\}$ satisfying $\hat{e}_k(e_j) = \delta_{jk}$. An alternative description is the following. For any $\alpha \in \mathcal{T}''^*$, let $Z''_\alpha \in \mathcal{T}''$ be defined by

$$L''(X, Z''_\alpha) = \alpha(X) \qquad \forall X \in \mathcal{T}''.$$

(This is possible, and Z''_α is unique, owing to the non-degeneracy of L''. Note that $\alpha \mapsto Z''_\alpha$ is conjugate-linear.) Then

$$\mathcal{L}(\alpha, \beta) = L''(Z''_\beta, Z''_\alpha) = \alpha(Z''_\beta) = \overline{\beta(Z''_\alpha)}.$$

Let, in particular, $Z''_f := Z''_{\overline{\partial}_b f}$, so that

$$L''(X, Z''_f) = \overline{\partial}_b f(X) \qquad \forall X \in \mathcal{T}'',$$

and denote by $Z'_f \in \mathcal{T}'$ the similarly defined holomorphic vector field satisfying

$$L'(Y, Z'_f) = \partial_b f(Y) \qquad \forall Y \in \mathcal{T}',$$

where $\partial_b f := df|_{\mathcal{T}'}$. Set

$$Z_f := i(\overline{Z''_f} - \overline{Z'_f}) \in \mathcal{T}' + \mathcal{T}''.$$

These objects are related to the symplectic structure of Σ as follows. Note that

$$d\eta = i\partial\overline{\partial} r = i \sum_{k,l=1}^{n} \frac{\partial^2 r}{\partial z_k \partial \overline{z}_l} \, dz_k \wedge d\overline{z}_l,$$

hence

$$d\eta(X' + X'', Y' + Y'') = iL'(X', \overline{Y''}) - iL'(Y', \overline{X''})$$

for all $X', Y' \in \mathcal{T}'$ and $X'', Y'' \in \mathcal{T}''$. It follows that $d\eta$ is a non-degenerate skew-symmetric bilinear form on $\mathcal{T}' + \mathcal{T}''$, and

$$d\eta(X, Z_f) = Xf \qquad \forall X \in \mathcal{T}' + \mathcal{T}''. \tag{17}$$

[1] or, perhaps more appropriately, a positive definite Hermitian *bivector*

Indeed,

$$\begin{aligned} d\eta(X'+X'',Z_f) &= iL'(X',\overline{-i\overline{Z'_f}}) - iL'(i\overline{Z''_f},\overline{X''}) \\ &= L'(X',Z'_f) + L''(X'',Z''_f) \\ &= \partial_b f(X') + \overline{\partial}_b f(X'') = df(X'+X''). \end{aligned}$$

Let us define $E_\mathcal{T} \in \mathcal{T}' + \mathcal{T}''$ by

$$d\eta(X,E_\mathcal{T}) = d\eta(X,E) \qquad \forall X \in \mathcal{T}'+\mathcal{T}'' \tag{18}$$

(again, this is possible and unambiguous by virtue of the non-degeneracy of $d\eta$ on $\mathcal{T}'+\mathcal{T}''$), and set

$$E_\perp := \frac{E-E_\mathcal{T}}{\eta(E)} = \frac{E-E_\mathcal{T}}{i\|\eta\|^2}.$$

The vector field $E_\perp$ is usually called the Reeb vector field, and is defined by the conditions $\eta(E_\perp)=1$, $i_{E_\perp}d\eta = 0$.

Proposition 7. *Let $f,g \in C^\infty(\partial\Omega)$, and let F,G be the functions on $\Sigma \cong \partial\Omega \times \mathbf{R}_+$ given by*

$$F(x,t) = t^{-k}f(x), \quad G(x,t) = t^{-m}g(x).$$

Then the Poisson bracket of F and G is given by

$$\{F,G\}_\Sigma = t^{-k-m-1}\Big(Z_f g + mgE_\perp f - kfE_\perp g\Big).$$

Proof. Recall that the Hamiltonian vector field H_F of F is the pre-dual of dF with respect to the symplectic form $\omega_\Sigma \equiv \omega$ on Σ, namely

$$\omega(X,H_F) = dF(X) = XF, \qquad \forall X \in \mathcal{T}\Sigma.$$

Since $F = t^{-k}f(x)$, we have $dF = t^{-k}df - kt^{-k-1}f\,dt$, so

$$H_F = t^{-k}H_f - kt^{-k-1}fH_t. \tag{19}$$

We claim that

$$H_t = E_\perp, \qquad H_f = \frac{1}{t}Z_f - E_\perp f\,T. \tag{20}$$

We check the formula for H_t, i.e.

$$\omega(X,H_t) = dt(X) \qquad \forall X \in \mathcal{T}\Sigma.$$

For $X = T$,

$$\begin{aligned}\omega(T, E_\perp) &= \frac{1}{\eta(E)}(td\eta + dt \wedge \eta)(T, E - E_\mathcal{T}) \\ &= \frac{1}{\eta(E)}\, dt \wedge \eta(T, E - E_\mathcal{T}) = \frac{\eta(E) - \eta(E_\mathcal{T})}{\eta(E)} \\ &= 1 = dt(T),\end{aligned}$$

since η vanishes on $\mathcal{T}' + \mathcal{T}'' \ni E_\mathcal{T}$. Similarly, for $X = X' \in \mathcal{T}'$,

$$\omega(X', E_\perp) = \frac{1}{\eta(E)}\, t\, d\eta(X', E_\perp)$$

vanishes by the definition (18) of $E_\mathcal{T}$, and so does $dt(E_\perp)$ since $E_\perp$ contains no t-differentiations. Analogously for $X = X'' \in \mathcal{T}''$. Finally, for $X = E$ we have

$$\begin{aligned}\omega(E, E_\perp) &= -\frac{1}{\eta(E)}\omega(E, E_\mathcal{T}) = -\frac{1}{\eta(E)}\, t\, d\eta(E, E_\mathcal{T}) \\ &= -\frac{1}{\eta(E)}\, t\, d\eta(E_\mathcal{T}, E_\mathcal{T}) = 0 = dt(E),\end{aligned}$$

where in the third equality we have used (18) for $X = E_\mathcal{T}$.
Next we check the formula for H_f. For $X = T$, both $\omega(X, H_f)$ and $df(X)$ are zero. For $X \in \mathcal{T}' + \mathcal{T}''$, we have $\omega(X, T) = dt \wedge \eta(X, T) = -\eta(X) = 0$ and the equality follows by (17). Finally for $X = E$

$$\begin{aligned}\omega(E, H_f) &= t\, d\eta(E, \tfrac{1}{t} Z_f) + dt \wedge \eta(E, -E_\perp f\, T) \\ &= d\eta(E_\mathcal{T}, Z_f) + \eta(E) E_\perp f \\ &= E_\mathcal{T} f + \eta(E) E_\perp f \qquad \text{by (17)} \\ &= E_\mathcal{T} f + (E - E_\mathcal{T}) f,\end{aligned}$$

which indeed coincides with $df(E) = Ef$.
By (20) and (19), we thus get

$$H_F = t^{-k-1} Z_f - t^{-k} E_\perp f\, T - kt^{-k-1} f E_\perp.$$

Consequently,

$$\begin{aligned}\{F, G\}_\Sigma &= \omega(H_F, H_G) = H_F G \\ &= t^{-k-m-1} Z_f g + mt^{-k-m-1} g E_\perp f - kt^{-k-m-1} f E_\perp g,\end{aligned}$$

and the assertion follows. □

Corollary 8. *Let $f, g \in C^\infty(\partial\Omega)$, and denote by f, g also the corresponding functions on $\Sigma \cong \partial\Omega \times \mathbf{R}_+$ constant on each fiber. Then*

$$\{f, g\}_\Sigma = \frac{1}{t} Z_f g = i\,\frac{\mathcal{L}(\overline{\partial}_b f, \overline{\partial}_b \overline{g}) - \mathcal{L}(\overline{\partial}_b g, \overline{\partial}_b \overline{f})}{t}.$$

Proof. Immediate upon taking $m = k = 0$ in the last proposition, and observing that

$$\begin{aligned} \frac{1}{i} Z_f g &= \overline{Z''_f} g - \overline{Z'_f} g = dg(\overline{Z''_f}) - dg(\overline{Z'_f}) \\ &= \partial_b g(\overline{Z''_f}) - \overline{\partial}_b g(\overline{Z'_f}) = \overline{\overline{\partial}_b \overline{g}(Z''_f)} - \overline{\partial}_b g(\overline{Z'_f}) \\ &= \overline{\mathcal{L}(\overline{\partial}_b \overline{g}, \overline{\partial}_b f)} - \mathcal{L}(\overline{\partial}_b g, \overline{\partial}_b \overline{f}), \end{aligned}$$

since $\overline{Z'_f} = Z''_{\overline{f}}$ by virtue of (16). □

We are now ready to state the main result of this section and, in some sense, of this paper.

Theorem 9. *Let U, W have the same meaning as in Proposition 2. Then for $f, g \in C^\infty(\overline{\Omega})$,*

$$U^*(\mathbf{T}_{f\overline{g}} - \mathbf{T}_{\overline{g}}\mathbf{T}_f)U = W T_Q W^*,$$

where T_Q is a generalized Toeplitz operator on $\partial\Omega$ of order -1 with principal symbol

$$\sigma(T_Q)(x, t\eta_x) = \frac{1}{t}\,\mathcal{L}(\overline{\partial}_b f, \overline{\partial}_b g)(x). \tag{21}$$

Proof. By Proposition 2,

$$U^*(\mathbf{T}_{f\overline{g}} - \mathbf{T}_{\overline{g}}\mathbf{T}_f)U = W(T_{Q_{f\overline{g}}} - T_{Q_{\overline{g}}} T_{Q_f})W^*,$$

where $T_{Q_f} = T_\Lambda^{-1/2} T_{\Lambda_f} T_\Lambda^{-1/2}$ is a generalized Toeplitz operator of order 0 with symbol $\sigma(T_{Q_f})(x, \xi) = f(x)$. By (P1) and (P4), the expression $T_{Q_{f\overline{g}}} - T_{Q_{\overline{g}}} T_{Q_f}$ is thus a generalized Toeplitz operator T_Q of order 0 with symbol $\sigma(T_Q) = \sigma(T_{Q_{f\overline{g}}}) - \sigma(T_{Q_{\overline{g}}})\sigma(T_{Q_f}) = f\overline{g} - \overline{g}f = 0$; thus by (P6), it is indeed, in fact, a generalized Toeplitz operator of order -1. It remains to show that its symbol, which we denote by $\rho(f, g)$, is given by (21).

By the general theory, $\rho(f, g)$ is given by a local expression, i.e. one involving only finitely many derivatives of f and g at the given point, and linear in f and $\overline{g}$. (Indeed, the proof of Proposition 2.5 in [5] shows that the construction, for a given ΨDO Q, of the ΨDO P from property (P2), i.e. such that $T_Q = T_P$ and $[P, \Pi] = 0$, is completely local in nature, so the total symbol of the P corresponding to $Q = \Lambda_f$ is given by local expressions in terms of the total symbol of Λ_f, hence, by local expressions in terms of f; the claim thus follows from the product formula for the symbol of ΨDOs.) It is therefore enough to show that

$$\rho(f,g)=\frac{1}{t}\mathcal{L}(\overline{\partial}_b f,\overline{\partial}_b g) \tag{22}$$

for functions f,g of the form $u\overline{v}$, with u,v holomorphic on $\overline{\Omega}$. [2] Next, if u and v are holomorphic on $\overline{\Omega}$, then $\mathbf{T}_{\overline{v}}\mathbf{T}_f=\mathbf{T}_{\overline{v}f}$ and $\mathbf{T}_f\mathbf{T}_u=\mathbf{T}_{fu}$ for any f; consequently, using Proposition 2 and (11),

$$\begin{aligned}
U^*(\mathbf{T}_{uf\overline{vg}}-\mathbf{T}_{\overline{vg}}\mathbf{T}_{uf})U&=U^*\mathbf{T}_{\overline{v}}(\mathbf{T}_{f\overline{g}}-\mathbf{T}_{\overline{g}}\mathbf{T}_f)\mathbf{T}_uU\\
&=U^*\mathbf{T}_{\overline{v}}UU^*(\mathbf{T}_{f\overline{g}}-\mathbf{T}_{\overline{g}}\mathbf{T}_f)UU^*\mathbf{T}_uU\\
&=WT_{Q_{\overline{v}}}W^*W(T_{Q_{f\overline{g}}}-T_{Q_{\overline{g}}}T_{Q_f})W^*WT_{Q_u}W^*\\
&=WT_{Q_{\overline{v}}}(T_{Q_{f\overline{g}}}-T_{Q_{\overline{g}}}T_{Q_f})T_{Q_u}W^*.
\end{aligned}$$

By (P4) we see that

$$\rho(uf,vg)=u\,\rho(f,g)\,\overline{v}.$$

Since also

$$\mathcal{L}(\overline{\partial}_b uf,\overline{\partial}_b vg)=u\,\mathcal{L}(\overline{\partial}_b f,\overline{\partial}_b g)\,\overline{v}$$

(because $\overline{\partial}_b(uf)=u\,\overline{\partial}_b f$ for holomorphic u), it in fact suffices to prove (22) when f,g are both conjugate-holomorphic, i.e. $\overline{\partial}_b\overline{f}=\overline{\partial}_b\overline{g}=0$. However, in that case $\mathbf{T}_{f\overline{g}}=\mathbf{T}_f\mathbf{T}_{\overline{g}}$, so, using again Proposition 2 and (11),

$$\begin{aligned}
U^*(\mathbf{T}_{f\overline{g}}-\mathbf{T}_{\overline{g}}\mathbf{T}_f)U&=U^*[\mathbf{T}_f,\mathbf{T}_{\overline{g}}]U=[U^*\mathbf{T}_fU,U^*\mathbf{T}_{\overline{g}}U]\\
&=[WT_{Q_f}W^*,WT_{Q_{\overline{g}}}W^*]=W[T_{Q_f},T_{Q_{\overline{g}}}]W^*,
\end{aligned}$$

implying that

$$\begin{aligned}
\rho(f,g)&=\sigma([T_{Q_f},T_{Q_{\overline{g}}}])\\
&=\tfrac{1}{i}\{\sigma(T_{Q_f}),\sigma(T_{Q_{\overline{g}}})\}_\Sigma\\
&=\tfrac{1}{i}\{f,\overline{g}\}_\Sigma\\
&=\frac{\mathcal{L}(\overline{\partial}_b f,\overline{\partial}_b g)-\mathcal{L}(\overline{\partial}_b\overline{g},\overline{\partial}_b\overline{f})}{t}\qquad\text{by Corollary 8}\\
&=\tfrac{1}{t}\,\mathcal{L}(\overline{\partial}_b f,\overline{\partial}_b g),
\end{aligned}$$

completing the proof. □

Remark 10. It seems much more difficult to obtain a formula for the symbol of $T_{PQ}-T_PT_Q$ for general ΨDOs P and Q. □

We are now ready to prove the main result on Dixmier traces.

[2] In fact, even holomorphic polynomials u,v would do.

Theorem 11. *Let $f_1, g_1, \dots, f_n, g_n \in C^\infty(\overline{\Omega})$. Then the operator*

$$H = H^*_{g_1} H_{f_1} H^*_{g_2} H_{f_2} \dots H^*_{g_n} H_{f_n}$$

on $L^2_{\mathrm{hol}}(\Omega)$ belongs to the Dixmier class, and

$$\mathrm{Tr}_\omega(H) = \frac{1}{n!(2\pi)^n} \int_{\partial\Omega} \mathcal{L}(\overline{\partial}_b f_1, \overline{\partial}_b g_1) \dots \mathcal{L}(\overline{\partial}_b f_n, \overline{\partial}_b g_n)\, \eta \wedge (d\eta)^{n-1}. \tag{23}$$

In particular, H is measurable.

Proof. Denote, for brevity, $V_j := T_\Lambda^{-1/2}(T_{\Lambda_{f_j \overline{g}_j}} - T_{\Lambda_{\overline{g}_j}} T_\Lambda^{-1} T_{\Lambda_{f_j}}) T_\Lambda^{-1/2}$. We have seen in the last theorem that $H^*_{g_j} H_{f_j} = \mathbf{T}_{\overline{g}_j f_j} - \mathbf{T}_{\overline{g}_j} \mathbf{T}_{f_j}$ satisfies

$$U^* H^*_{g_j} H_{f_j} U = W V_j W^*$$

and that V_j is a generalized Toeplitz operator of order -1 with symbol given by $\sigma(V_j)(x, t\eta_x) = \frac{1}{t} \mathcal{L}(\overline{\partial}_b f_j, \overline{\partial}_b g_j)$. By iteration and using (11), it follows that

$$U^* H^*_{g_1} H_{f_1} H^*_{g_2} H_{f_2} \dots H^*_{g_n} H_{f_n} U = W V_1 V_2 \dots V_n W^* = W V W^*,$$

where $V := V_1 V_2 \dots V_n$ is a generalized Toeplitz operator of order $-n$ with symbol $\sigma(V)(x, t\eta_x) = t^{-n} \prod_{j=1}^n \mathcal{L}(\overline{\partial}_b f_j, \overline{\partial}_b g_j)$. An application of Theorem 3 completes the proof. $\square$

Corollary 12. *Let f be holomorphic on Ω and C^∞ on $\overline{\Omega}$. Then $|H_{\overline{f}}|^{2n}$ is in the Dixmier class, measurable, and*

$$\mathrm{Tr}_\omega(|H_{\overline{f}}|^{2n}) = \frac{1}{n!(2\pi)^n} \int_{\partial\Omega} \mathcal{L}(\overline{\partial}_b \overline{f}, \overline{\partial}_b \overline{f})^n\, \eta \wedge (d\eta)^{n-1}.$$

By standard matrix algebra, one has[3]

$$\mathcal{L}(\overline{\partial}_b f, \overline{\partial}_b g) = \begin{bmatrix} \overline{\partial}\tilde{g} \\ 0 \end{bmatrix}^* \begin{bmatrix} \partial\overline{\partial} r & \overline{\partial} r \\ \partial r & 0 \end{bmatrix}^{-1} \begin{bmatrix} \overline{\partial}\tilde{f} \\ 0 \end{bmatrix},$$

[3]Let, quite generally, X be an operator on $\mathbf{C}^n$, $u \in \mathbf{C}^n$, and denote by A the compression of X to the orthogonal complement $u^\perp$ of u, i.e. $A = PX|_{\mathrm{Ran}\, P}$ where $P : \mathbf{C}^n \to u^\perp$ is the orthogonal projection. Assume that A is invertible. Then the block matrix $\begin{bmatrix} X & u \\ u^* & 0 \end{bmatrix} \in \mathbf{C}^{(n+1)\times(n+1)}$ is invertible, and for any $v, w \in \mathbf{C}^n$,

$$\langle A^{-1} P v, P w \rangle = \begin{bmatrix} w \\ 0 \end{bmatrix}^* \begin{bmatrix} X & u \\ u^* & 0 \end{bmatrix}^{-1} \begin{bmatrix} v \\ 0 \end{bmatrix}.$$

Indeed, switching to a convenient basis we may assume that $u = [0, \dots, 0, 1]^t$. Write $X = \begin{bmatrix} A & b \\ c^* & d \end{bmatrix}$, with $b, c \in \mathbf{C}^n$, $d \in \mathbf{C}$. Then

$$\begin{bmatrix} X & u \\ u^* & 0 \end{bmatrix} = \begin{bmatrix} A & b & 0 \\ c^* & d & 1 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & b \\ 0 & 1 & d \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} A & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ c^* & 0 & 1 \end{bmatrix},$$

where $\tilde f, \tilde g$ are any smooth extensions of $f, g \in C^\infty(\partial\Omega)$ to a neighbourhood of $\partial\Omega$.
In particular, for $\Omega = \mathbf{B}^d$, the unit ball, with the defining function $r(z) = |z|^2 - 1$, we obtain

$$\mathcal{L}(\overline\partial_b f, \overline\partial_b g) = \sum_{j=1}^n \frac{\partial \tilde f}{\partial \overline z_j} \overline{\frac{\partial \tilde g}{\partial \overline z_j}} - \overline R \tilde f \overline{\overline R \tilde g}, \tag{24}$$

where $\overline R := \sum_{j=1}^n \overline z_j \frac{\partial}{\partial \overline z_j}$ is the anti-holomorphic radial derivative. One also easily checks that $\eta \wedge (d\eta)^{n-1} = (2\pi)^n \, d\sigma$ where $d\sigma$ is the normalized surface measure on $\partial \mathbf{B}^n$. The last two theorems thus recover, as they should, the results from [12] (Theorem 4.4 — which is the formula (3) above — and Corollary 4.5 there).
Note also that for $n = 1$, the expression (24) vanishes; in this case $U^* H_g^* H_f U$ is thus in fact of order not -1 but -2 (so that $|H_g^* H_f|^{1/2}$ is in the Dixmier class rather than $H_g^* H_f$), and some additional work is needed to compute the symbol (and, from it, the Dixmier trace); see [13].
Finally, we pause to remark that the value of the integral (23) remains unchanged under biholomorphic mappings, as well as changes of the defining function. Indeed, if r is replaced by gr, with $g > 0$ on $\partial\Omega$, then $\mathcal{T}''$ and $\overline\partial_b$ are unaffected, while the Levi form L on $\mathcal{T}''$ gets multiplied by g. Hence its dual $\mathcal{L}$ gets multiplied by g^{-1}, and as $\eta \wedge (d\eta)^{n-1}$ transforms into $g^n \eta \wedge (d\eta)^{n-1}$ (cf. Remark 4), the integrand in (23) does not change. Similarly, if $\phi : \Omega_1 \to \Omega_2$ is a biholomorphic map and r is a defining function for Ω_2, one can choose $\phi \circ r$ as the defining function for Ω_1; then it is immediate, in turn, that ϕ sends $\mathcal{T}'$ into $\mathcal{T}'$ and $\mathcal{T}''$ into $\mathcal{T}''$, and that it transforms each of η, $\eta \wedge (d\eta)^{n-1}$, $\overline\partial_b$, ∂_b, L and $\mathcal{L}$ into the corresponding object on the other domain. Hence $\mathcal{L}(\overline\partial_b f, \overline\partial_b g) = (\phi_* \mathcal{L})(\phi^* \overline\partial_b f, \phi^* \overline\partial_b g) = \mathcal{L}(\overline\partial_b (f \circ \phi), \overline\partial_b (g \circ \phi))$ and, finally, $\phi^*(\prod_j \mathcal{L}(\overline\partial_b f_j, \overline\partial_b g_j) \, \eta \wedge (d\eta)^{n-1}) = \prod_j \mathcal{L}(\overline\partial_b (f_j \circ \phi), \overline\partial_b (g_j \circ \phi)) \, \eta \wedge (d\eta)^{n-1}$, proving the claim. Note that e.g. even in the formula (3) for $\Omega = \mathbf{B}^n$, the invariance of the value of the integral under biholomorphic self-maps of the ball is definitely not apparent.

5. Concluding remarks

5.1 Manifolds. The results in this paper should all be generalizable to arbitrary strictly pseudoconvex manifolds.

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whence

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ c^* & 0 & 1 \end{bmatrix} \begin{bmatrix} X & u \\ u^* & 0 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & b \\ 0 & 1 & d \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} A & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

and the claim follows.
The formula for $\mathcal{L}(\overline\partial_b f, \overline\partial_b g)$ is obtained upon taking $X = \mathbb{L}$, $u = \overline\partial r$, $v = \overline\partial f$ and $w = \overline\partial g$.

5.2 Residual trace. Comparing Theorem 3 with the results of Guillemin [16] [17], we see that the Dixmier trace for generalized Toeplitz operators coincides (possibly up to different normalization) with the residual trace of Wodzicki, Guillemin, Manin and Adler. This is completely analogous to the situation for ΨDOs, cf. Connes [8], Theorem 1.

5.3 Nonsmooth symbols. For the unit disc $\mathbf{D}$ in $\mathbf{C}$, the analogue of Corollary 12 is

$$\operatorname{Tr}_\omega(|H_{\overline{f}}|) = \int_{\partial\mathbf{D}} |f'(e^{i\theta})| \, \frac{d\theta}{2\pi}$$

for f holomorphic on $\mathbf{D}$ and smooth on $\overline{\mathbf{D}}$; see [13]. It was shown in [13] that the smoothness assumption can be dispensed with: namely, for f holomorphic on $\mathbf{D}$, $|H_{\overline{f}}| \in \mathcal{S}^{\mathrm{Dixm}}$ if and only if f' belongs to the Hardy 1-space $H^1(\partial\mathbf{D})$, and then

$$\operatorname{Tr}_\omega(|H_{\overline{f}}|) = \|f'\|_{H^1}.$$

We expect that the same situation prevails also for general domains Ω of the kind studied in this paper, in the following sense. For f holomorphic on Ω, denote

$$\mathcal{L}_f(z) := \begin{bmatrix} \partial f \\ 0 \end{bmatrix}^* \begin{bmatrix} \partial\overline{\partial} r & \partial r \\ \overline{\partial} r & 0 \end{bmatrix}^{-1} \begin{bmatrix} \partial f \\ 0 \end{bmatrix} (z).$$

This is a smooth function defined in some neighbourhood of $\partial\Omega$ in $\overline{\Omega}$, whose boundary values coincide with $\mathcal{L}(\overline{\partial}_b \overline{f}, \overline{\partial}_b \overline{f})$ if f is smooth up to the boundary.

Conjecture. *Let f be holomorphic on Ω. Then $|H_{\overline{f}}|^{2n} \in \mathcal{S}^{\mathrm{Dixm}}$ if and only if*

$$\|f\|_{\mathcal{L}} := \limsup_{\epsilon \searrow 0} \Big(\frac{1}{n!(2\pi)^n} \int_{r=-\epsilon} |\mathcal{L}_f|^n \, |\eta \wedge (d\eta)^{n-1}| \Big)^{1/2n}$$

is finite, and then

$$\operatorname{Tr}_\omega(|H_{\overline{f}}|^{2n}) = \|f\|_{\mathcal{L}}^{2n}.$$

The proof for the disc went by showing first that $\|f'\|_{H_1}$ actually dominates the $\mathcal{S}^{\mathrm{Dixm}}$ norm of $|H_{\overline{f}}|$; the result then followed from the one for $f \in C^\infty(\overline{\mathbf{D}})$ by a straightforward approximation argument. This approach might also work for general domains Ω (with $\|f\|_{\mathcal{L}}$ and $|H_{\overline{f}}|^{2n}$ replacing $\|f'\|_{H^1}$ and $|H_{\overline{f}}|$), but the techniques for doing so (estimates for the oscillation of f' on Carleson-type rectangles, etc.) are outside the scope of this paper.

5.4 Higher type. The generalized Toeplitz operators on $H^2(\partial\Omega)$ of *higher type* m, $m = 1, 2, \dots$, are defined as $T_Q^{(m)} = \Pi_m Q \Pi_m$, where Q is a ΨDO on $\partial\Omega$ as before and Π_m is the orthogonal projection in $L^2(\partial\Omega)$ onto the subspace $H^2_{(m)}(\partial\Omega)$ of functions annihilated by the m-th symmetric power of $\overline{\partial}_b$; in other words,

$$H^2_{(m)}(\partial\Omega) = \text{closure of } \{f \in C^\infty(\partial\Omega) : \overline{R}_{j_1} \overline{R}_{j_2} \dots \overline{R}_{j_m} f = 0 \ \forall j_1, j_2, \dots, j_m\}.$$

For $m = 1$, this recovers the ordinary Szegö projector Π and the generalized Toeplitz operators discussed so far. As shown in §15.3 of [5], the projectors Π_m have almost the same microlocal description as Π, so it is conceivable that our results could also be extended to these higher type Toeplitz operators.

5.5 Weighted spaces. Our methods also work, with only minimal modifications, for $L^2_{\text{hol}}(\Omega)$ replaced by the weighted Bergman spaces $L^2_{\text{hol}}(\Omega, |r|^\nu) \subset L^2(\Omega, |r|^\nu)$, with any $\nu > -1$. The formulas in Theorems 9 and 11, and in Corollary 12, remain unchanged (i.e. they do not depend on ν).
Finally, it is immediate from Theorem 3, the property (P4) and the proof of Theorem 9 that the formulas in Theorem 11 and Corollary 12 also remain valid for Hankel operators on the Hardy space $H^2(\partial\Omega)$.

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Galois Representations Attached to Hilbert-Siegel Modular Forms

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Abstract. This article is a spinoff of the book of Harris and Taylor [HT], in which they prove the local Langlands conjecture for $\mathrm{GL}(n)$, and its companion paper by Taylor and Yoshida [TY] on local-global compatibility. We record some consequences in the case of genus two Hilbert-Siegel modular forms. In other words, we are concerned with cusp forms π on $\mathrm{GSp}(4)$ over a totally real field, such that π_∞ is regular algebraic (that is, π is cohomological). When π is globally generic (that is, has a non-vanishing Fourier coefficient), and π has a Steinberg component at some finite place, we associate a Galois representation compatible with the local Langlands correspondence for $\mathrm{GSp}(4)$ defined by Gan and Takeda in a recent preprint [GT]. Over $\mathbb{Q}$, for π as above, this leads to a new realization of the Galois representations studied previously by Laumon, Taylor and Weissauer. We are hopeful that our approach should apply more generally, once the functorial lift to $\mathrm{GL}(4)$ is understood, and once the so-called book project is completed. An application of the above compatibility is the following special case of a conjecture stated in [SU]: If π has nonzero vectors fixed by a non-special maximal compact subgroup at v, the corresponding monodromy operator at v has rank at most one.

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1 Introduction

The interplay between modular forms and Galois representations has shown to be extremely fruitful in number theory. For example, the Hasse-Weil conjecture, saying that the L-function of an elliptic curve over $\mathbb{Q}$ has meromorphic continuation to $\mathbb{C}$, was proved in virtue of this reciprocity. Some of the most basic examples are Hilbert modular forms and Siegel modular forms, both very well-studied in the literature. In this paper, we study a mixture of these. First, we introduce the Siegel upper half-space (of complex dimension three):

$$\mathcal{H} \overset{\text{df}}{=} \{Z = X + iY \in M_2(\mathbb{C}) \text{ symmetric, with } Y \text{ positive definite}\}.$$

For a moment, we will view the symplectic similitude group GSp(4) as an affine group scheme over $\mathbb{Z}$, by choosing the non-degenerate alternating form to be

$$\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Later, beyond this introduction, we will switch to a skew-diagonal form. The similitude character is denoted by c throughout. We then consider the subgroup $\mathrm{GSp}(4,\mathbb{R})^+$ of elements with positive similitude. It acts on $\mathcal{H}$ in the standard way, by linear fractional transformations. More precisely, by the formula:

$$gZ = (AZ+B)(CZ+D)^{-1}, \quad g = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathrm{GSp}(4,\mathbb{R})^+, \quad Z \in \mathcal{H}.$$

The automorphy factor $CZ+D$ will be denoted by $j(g,Z)$ from now on. Next, we look at the d-fold product of this setup. In more detail, we will concentrate on a discrete subgroup Γ inside $\mathrm{GSp}(4,\mathbb{R})^{+d}$, and its diagonal action on $\mathcal{H}^d$. To exhibit examples of such Γ, we bring into play a totally real number field F, of degree d over $\mathbb{Q}$, and label the real embeddings by σ_i. This ordering is used to identify $\mathrm{GSp}(4,\mathcal{O})^+$ with a discrete subgroup Γ. Here the plus signifies that we look at elements whose similitude is a totally positive unit in $\mathcal{O}$, the ring of integers in F. Finally, in order to define modular forms for Γ, we fix weights

$$\underline{k}_i = (k_{i,1}, k_{i,2}), \quad k_{i,1} \geq k_{i,2} \geq 3, \quad i = 1, \ldots, d.$$

For each i, introduce the irreducible algebraic representation $\rho_{\underline{k}_i}$ of $\mathrm{GL}(2,\mathbb{C})$,

$$\mathrm{Sym}^{k_{i,1}-k_{i,2}}(\mathbb{C}^2) \otimes \det{}^{k_{i,2}}.$$

The underlying space of $\rho_{\underline{k}_i}$ is just a space of polynomials in two variables, homogeneous of a given degree. Following [Bai], we then define a Hilbert-Siegel modular form for Γ, with weights $\underline{k}_i$, to be a holomorphic vector-valued function

$$f : \mathcal{H}^d \to \bigotimes_{i=1}^{d} \mathrm{Sym}^{k_{i,1}-k_{i,2}}(\mathbb{C}^2) \otimes \det{}^{k_{i,2}}$$

satisfying the following transformation property for every $\underline{Z} \in \mathcal{H}^d$ and $\gamma \in \Gamma$:

$$f(\gamma \underline{Z}) = \bigotimes_{i=1}^{d} \rho_{\underline{k}_i}(c(\gamma_i)^{-1} j(\gamma_i, Z_i)) \cdot f(\underline{Z}).$$

Such f are automatically holomorphic at infinity, by the Koecher principle. The form is often assumed to be cuspidal, that is, it vanishes at infinity. These modular forms have rich arithmetic properties. To exploit them, it is useful to switch to an adelic setup and instead look at automorphic representations. For instance, this immediately gives rise to a workable Hecke theory. Thus, from now on in this paper, instead of f we will focus on a cuspidal automorphic representation π of GSp(4) over the totally real field F. The analogues of Hilbert-Siegel modular forms are those π which are holomorphic discrete series at infinity. It is a basic fact that such π do *not* admit Whittaker models. However, it is generally believed that the L-function of π coincides with the L-function of a π' which *does* admit a Whittaker model. Hence, for our purposes, there is no serious harm in assuming the existence of such a model. For a while though, let us not make this assumption, and explain in detail the expectations regarding Hilbert-Siegel modular forms and their associated Galois representations.

Let π be a cuspidal automorphic representation of GSp(4) over some totally real field F, and denote by S_π the set of finite places where π is ramified. For each infinite place v, we assume that π_v is an essentially discrete series representation, and that π_v has central character $a \mapsto a^{-w}$. Here w is an integer, independent of v. Under these assumptions, and a choice of an isomorphism $\iota : \bar{\mathbb{Q}}_\ell \to \mathbb{C}$, it is expected that there should be a semisimple continuous Galois representation

$$\rho_{\pi,\iota} : \mathrm{Gal}(\bar{F}/F) \to \mathrm{GL}_4(\bar{\mathbb{Q}}_\ell)$$

with the following properties: $\rho_{\pi,\iota}$ is unramified at $v \notin S_\pi$ not dividing ℓ, and

$$L_v(s - \frac{3}{2}, \pi, \mathrm{spin}) = \det(1 - \iota\rho_{\pi,\lambda}(\mathrm{Frob}_v) \cdot q_v^{-s})^{-1}.$$

Here Frob_v is the geometric Frobenius. More prudently, the above spin L-factor should actually lie in $L[q_v^{-s}]$ for some number field L inside $\mathbb{C}$, and instead of ι one could focus on the finite place of L it defines. In the *rational* case $F = \mathbb{Q}$, the existence of $\rho_{\pi,\iota}$ is now known, due to the work of many people (Chai-Faltings, Laumon, Shimura, Taylor and Weissauer). See [Lau] and [Wei] for the complete result. For arbitrary F, not much is known. Of course, when π is CAP (cuspidal associated to parabolic), or a certain functorial lift (endoscopy, base change or automorphic induction), $\rho_{\pi,\iota}$ is known to exist by [BRo]. However, in most of these cases $\rho_{\pi,\iota}$ is reducible. In the opposite case, that is, when π genuinely belongs to GSp(4), the representation $\rho_{\pi,\iota}$ should be irreducible. Obviously, this is the case we are interested in. Actually, we will aim higher and consider the ramified places S_π too. The impetus for doing so, is the recent work of Gan and Takeda [GT], in which they prove the local Langlands conjecture for GSp(4). To an irreducible admissible representation π_v, they associate an L-parameter

$$\mathrm{rec}_{\mathrm{GT}}(\pi_v) : W'_{F_v} = W_{F_v} \times \mathrm{SL}(2,\mathbb{C}) \to \mathrm{GSp}(4,\mathbb{C}).$$

The notation $\mathrm{rec}_{\mathrm{GT}}$ is ours. This correspondence is natural in a number of respects. For example, it preserves the L- and ϵ-factors defined by Shahidi in the generic case [Sha]. See section 2.2.2 below for a discussion of the complete list of desiderata. Now, the representation $\rho_{\pi,\iota}$ should satisfy local-global compatibility. That is, for any finite place v (not dividing ℓ), the restriction $\rho_{\pi,\iota}|_{W_{F_v}}$ should correspond to $\mathrm{rec}_{\mathrm{GT}}(\pi_v)$ through the usual dictionary [Tat]. As it stands, this is only morally true; one has to twist π_v. The precise folklore prediction is:

Conjecture. *Let π be a cuspidal automorphic representation of GSp(4) over some totally real field F. Assume there is a cuspidal automorphic representation of GL(4) over F, which is a weak lift of π. Moreover, we assume that*

$$\pi^\circ \overset{df}{=} \pi \otimes |c|^{\frac{w}{2}} \text{ is unitary, for some } w \in \mathbb{Z}.$$

Finally, at each infinite place v, we assume that π_v is an essentially discrete series representation with the same central and infinitesimal character as the finite-dimensional irreducible algebraic representation $V_{\mu(v)}$ of highest weight

$$t = \begin{pmatrix} t_1 & & & \\ & t_2 & & \\ & & t_3 & \\ & & & t_4 \end{pmatrix} \mapsto t_1^{\mu_1(v)} t_2^{\mu_2(v)} c(t)^{\delta(v)-w}, \quad \delta(v) \overset{df}{=} \frac{1}{2}(w - \mu_1(v) - \mu_2(v)).$$

Here $\mu_1(v) \geq \mu_2(v) \geq 0$ are integers such that $\mu_1(v)+\mu_2(v)$ has the same parity as w. In particular, the central character ω_{π_v} is of the form $a \mapsto a^{-w}$ at each infinite place v. Under these assumptions, for each choice of an isomorphism $\iota : \bar{\mathbb{Q}}_\ell \to \mathbb{C}$, there is a unique irreducible continuous representation

$$\rho_{\pi,\iota} : Gal(\bar{F}/F) \to GSp_4(\bar{\mathbb{Q}}_\ell)$$

characterized by the following property: For each finite place $v \nmid \ell$ of F, we have

$$\iota WD(\rho_{\pi,\iota}|_{W_{F_v}})^{F-ss} \simeq rec_{GT}(\pi_v \otimes |c|^{-\frac{3}{2}}).$$

Moreover, π° is tempered everywhere. Consequently, $\rho_{\pi,\iota}$ is pure of weight $\mathbf{w} \overset{df}{=} w+3$. The representation $\rho_{\pi,\iota}$ has the following additional properties:

- $\rho_{\pi,\iota}^\vee \simeq \rho_{\pi,\iota} \otimes \chi^{-1}$ *where the similitude character $\chi = \omega_{\pi^\circ} \cdot \chi_{cyc}^{-\mathbf{w}}$ is totally odd.*
- *The representation $\rho_{\pi,\iota}$ is potentially semistable at any finite place $v|\ell$. Moreover, $\rho_{\pi,\iota}$ is crystalline at a finite place $v|\ell$ when π_v is unramified.*

- *The Hodge-Tate weights are given by the following recipe: Fix an infinite place v, and use the same notation for the place above ℓ it defines via ι.*

$$\dim_{\bar{\mathbb{Q}}_\ell} gr^j(\rho_{\pi,\iota} \otimes_{F_v} B_{dR})^{Gal(\bar{F}_v/F_v)} = 0,$$

unless j belongs to the set

$$\delta(v) + \{0, \mu_2(v)+1, \mu_1(v)+2, \mu_1(v)+\mu_2(v)+3\},$$

in which case the above dimension is equal to one.

The notation used will be explained carefully in the main body of the text below. Our main result is a proof of this conjecture in a substantial number of cases. The depth (and the Swan conductor) are defined below in Section 4.5, as is J_Q.

Main Theorem.

(a) *The above conjecture holds for globally generic π such that, for some finite place v, the local component π_v is an unramified twist of the Steinberg representation.*

(b) *Let $\rho_{\pi,\iota}$ be the Galois representation attached to a globally generic cusp form π as in part (a). Let $v \nmid \ell$ be a finite place of F such that π_v is Iwahori-spherical and ramified. Then $\rho_{\pi,\iota}|_{I_{F_v}}$ acts unipotently. Moreover,*

- *π_v of Steinberg type $\Longleftrightarrow$ monodromy has rank 3.*
- *π_v has a unique J_Q-fixed line $\Longleftrightarrow$ monodromy has rank 2.*
- *π_v para-spherical $\Longleftrightarrow$ monodromy has rank 1.*

(c) *Let $\rho_{\pi,\iota}$ be the Galois representation attached to a globally generic cusp form π as in part (a). Let $v \nmid \ell$ be a finite place of F such that π_v is supercuspidal, and not a lift from $GO(2,2)$. Then $\rho_{\pi,\iota}|_{W_{F_v}}$ is irreducible. Furthermore, $\rho_{\pi,\iota}$ is trivial on some finite index subgroup of I_{F_v}, and*

$$\mathfrak{f}_{Swan}(\rho_{\pi,\iota}|_{I_{F_v}}) = 4 \cdot depth(\pi_v).$$

Part of our original motivation for writing this paper, was to determine the rank of the monodromy operator for $\rho_{\pi,\iota}$ at a place v where π_v is Iwahori-spherical (that is, has nonzero vectors fixed by an Iwahori-subgroup). The question is completely answered by part (b). Here J_Q denotes the Klingen parahoric, and by π_v being *para-spherical* we mean that it has nonzero vectors fixed by a non-special maximal compact subgroup. The first two statements in (b) are part of the Conjecture on p. 11 in [GTi], while the latter statement in (b) is part of Conjecture 3.1.7 on p. 41 in [SU]. The holomorphic analogue of the latter would have applications to the Bloch-Kato conjecture for modular forms of square-free level. See [SU] and the authors thesis [Sor].

The proof of part (b) essentially follows from the local-global compatibility from part (a), and the classification of the Iwahori-spherical representations of GSp(4). The dimensions of the parahoric fixed spaces for each class of representations were tabulated in [Sch]. We only need the generic ones. For those six types of representations, the data are reproduced in Table A in section 4.5 below.

The proof of part (a) is an application of the monumental work of Harris-Taylor [HT], and its refinement by Taylor-Yoshida [TY]. Let us briefly sketch the simple strategy: First, since π is globally generic, one can lift it to an automorphic representation Π on GL(4) using theta series, by utilizing the close connection with $GO(3,3)$. This is a well-known, though unpublished, result of Jacquet, Piatetski-Shapiro and Shalika. Other proofs exist in the literature. For example, see [AS] for an approach using the converse theorem. We make use of Theorem 13.1 in [GT], saying that the lift $\pi \mapsto \Pi$ is strong. That is, compatible with the local Langlands correspondence everywhere. We note that, by the Steinberg assumption, Π must be cuspidal. Next, we base change Π to a CM extension E over F, and twist it by a suitable character χ to make it conjugate self-dual. We can now apply [HT] and [TY] to the representation $\Pi_E(\chi)$, in order to get a Galois representation $\rho_{\Pi_E(\chi),\iota}$ over E. Since E is arbitrary, a delicate patching argument shows how to descend this collection to F, after twisting by $\rho_{\check{\chi},\iota}$.

We note that the main theorem continues to hold if some π_v is a generalized Steinberg representation of Klingen type (see section 2 below), or a supercuspidal not coming from $GO(2,2)$. The point being that the local lift Π_v on GL(4) should remain a discrete series. However, eventually the book project of the Paris 7 GRFA seminar should make any local assumption at v superfluous. In fact, almost complete results of S.-W. Shin have been announced very recently (to pin down the *Frobenius* semisimplification, at the time of writing, one has to make a regularity assumption, which should be removable by a p-adic deformation argument). See Expected Theorem 2.4 in [Har]. Furthermore, the assumption that π is globally generic is used exclusively to get a strong lift to GL(4). Our understanding is that the current state of the trace formula should at least give a *weak* lift more generally. See [Art] in conjunction with [Whi]. In this respect, there is a very interesting preprint of Weissauer [We2], in which he proves that if π is a discrete series at infinity, it is weakly equivalent to a globally generic representation. However, apparently he needs to work over $\mathbb{Q}$. Perhaps ideas from [Lab] will be useful in treating F of degree at least two. In any case, to get a *strong* lift, one would have to show that the L-packets defined in [GT] satisfy the expected character relations. This seems to be quite difficult.

In part (c) we let $\mathfrak{f}_{\mathrm{Swan}}$ denote the Swan conductor, closely related to the more commonly used Artin conductor, and the depth of π_v is defined in [MP]. The precise definitions are recalled below in section 4.5. The proof of part (c) relies on two essential ingredients. One is a formula, due to Bushnell and Frolich [BF], relating the depth to the conductor in the case of supercuspidals on $\mathrm{GL}(n)$. The second is a paper of Pan, showing that the local theta correspondence preserves depth [Pan]. In particular, if π_v has depth zero, we deduce that $\rho_{\pi,\iota}$ is tamely ramified at v. We finish the paper with another criterion for tame ramification, due to Genestier and Tilouine [GTi] over $\mathbb{Q}$: Suppose $\pi_v^{J_Q,\chi}$ is nonzero, for some non-trivial character χ of $\mathbb{F}_v^*$ inflated to the units, then $\rho_{\pi,\iota}$ is tamely ramified:

$$\rho_{\pi,\iota}|_{I_{F_v}} = 1 \oplus 1 \oplus \chi \oplus \chi.$$

Here χ is the character of I_{F_v} obtained via local class field theory. Moreover, one can arrange for the two eigenspaces, for 1 and χ, to be totally isotropic.

From our construction of the compatible system $\rho_{\pi,\iota}$ in part (a), one deduces that it is *motivic* in the sense defined on p. 60 in [BRo]: There is a smooth projective variety $X_{/F}$, and an integer n, such that $\rho_{\pi,\iota}$ is a constituent of

$$H^j(X \times_F \bar{F}, \bar{\mathbb{Q}}_\ell)(n),$$

for all ℓ, where $\mathbf{w} = j - 2n$. By invoking the Weil restriction, it is enough to show the analogous result for $\rho_{\pi,\iota}|_{\Gamma_E}$ for some CM extension E over F. For a detailed argument, we refer to the proof of Proposition 5.2.1 on p. 86 in [BRo]. Over E, the variety is a self-product of the universal abelian variety over a simple Shimura variety. See the bottom isomorphism on p. 98 in [HT]. As in the case of Hilbert modular forms [BRo], one would like to have actual motives over E associated with π. Seemingly, one of the main obstacles in deriving this from [HT] is a multiplicity one issue for the unitary groups considered there: Is the positive integer a in part (6) on p. 12 of [TY] in fact equal to one? Conjecturally, one should even have motives over F attached to π. Even over $\mathbb{Q}$ this is not yet known. One problem is that the Hecke correspondences on a Siegel threefold do not extend to a given toroidal compactification. For a more thorough discussion of these matters, and a slightly different approach, see [H].

Many thanks are due to D. Ramakrishnan for his suggestion that I should look at the Hilbert-Siegel case by passing to a CM extension, and for sharing his insights on many occasions. I am also grateful to M. Harris for useful correspondence regarding the patching argument in section 4.3. Finally, I am thankful to C. Skinner and A. Wiles for discussions relevant to this paper, and for their encouragement and support.

2 Lifting to GL(4)

We will describe below how to transfer automorphic representations of $\mathrm{GSp}(4)$, of a certain type, to $\mathrm{GL}(4)$. Throughout, we work over a totally real base field F. Let us take π to be a globally generic cuspidal automorphic representation of $\mathrm{GSp}(4)$, with central character ω_π. We do *not* assume it is unitary. For $v|\infty$,

$$\pi_v \simeq \pi^W_{\mu(v)}, \quad \mu_1(v) \geq \mu_2(v) \geq 0, \quad \mu_1(v) + \mu_2(v) \equiv w \pmod 2.$$

The notation is explained more carefully below. Here we fix the integer w such that ω_{π_v} takes nonzero $a \mapsto a^{-w}$ for all archimedean places v. In particular,

$$\pi^\circ \overset{\mathrm{df}}{=} \pi \otimes |c|^{\frac{w}{2}} \textit{ is unitary.}$$

Using theta series, one can then associate an automorphic representation Π of $\mathrm{GL}(4)$ with the following properties: It has central character ω_π^2, and satisfies[1]

- $\Pi \otimes \omega_\pi^{-1} \simeq \Pi^\vee$.
- For $v|\infty$, the L-parameter of Π_v has the following restriction to $\mathbb{C}^*$,

$$z \mapsto |z|^{-w} \cdot \begin{pmatrix} (z/\bar{z})^{\frac{\nu_1+\nu_2}{2}} & & & \\ & (z/\bar{z})^{\frac{\nu_1-\nu_2}{2}} & & \\ & & (z/\bar{z})^{-\frac{\nu_1-\nu_2}{2}} & \\ & & & (z/\bar{z})^{-\frac{\nu_1+\nu_2}{2}} \end{pmatrix},$$

  where $\nu_1 = \mu_1 + 2$ and $\nu_2 = \mu_2 + 1$ give the Harish-Chandra parameter of π_v. Here we suppress the dependence on v, and simply write $\mu_i = \mu_i(v)$.
- $L(s, \Pi_v) = L(s, \pi_v, \mathrm{spin})$, for finite v such that π_v is unramified.

In fact, Gan and Takeda have recently defined a local Langlands correspondence for $\mathrm{GSp}(4)$ such that the above lift is *strong*. That is, the L-parameters of π_v and Π_v coincide at *all* places v. For later applications, we would like Π to have a square-integrable component. Using table 2 on page 51 in [GT], we can ensure this by assuming the existence of a finite place v_0 where π_{v_0} is of the form

$$\pi_{v_0} = \begin{cases} \mathrm{St}_{\mathrm{GSp}(4)}(\chi) \\ \mathrm{St}(\chi, \tau) \end{cases} \implies \Pi_{v_0} = \begin{cases} \mathrm{St}_{\mathrm{GL}(4)}(\chi) \\ \mathrm{St}(\tau). \end{cases}$$

Here $\mathrm{St}_{\mathrm{GSp}(4)}(\chi)$ is the Steinberg representation *twisted* by the character χ, which need not be unramified. Also, Π_{v_0} is supercuspidal if π_{v_0} is a supercuspidal not coming from $\mathrm{GO}(2,2)$. Most of the notation used here is self-explanatory, except maybe the symbol $\mathrm{St}(\chi, \tau)$: It denotes the generalized Steinberg representation, of Klingen type, associated to a supercuspidal τ on $\mathrm{GL}(2)$ and a non-trivial quadratic character χ such that $\tau \otimes \chi = \tau$. We refer to page 35 in [GT] for more details. As a bonus, the existence of such a place v_0 guarantees that Π is *cuspidal*: Otherwise, π is a theta lift from $\mathrm{GO}(2,2)$, but by [GT] the above π_{v_0} do not participate here.

2.1 The archimedean case

2.1.1 Discrete series for $\mathrm{GL}(2, \mathbb{R})$

In this section, we briefly set up notation for the discrete series representations of $\mathrm{GL}(2, \mathbb{R})$. Throughout we use Harish-Chandra parameters, as opposed to

[1] We normalize the isomorphism $W_{\mathbb{R}}^{\mathrm{ab}} \simeq \mathbb{R}^*$ using the absolute value $|z|_{\mathbb{C}} \overset{\mathrm{df}}{=} |z|^2$.

Blattner parameters. We will follow the notation of [Lau]. Thus, for each positive integer n, we let σ_n be the unique (essentially) discrete series representation of $\mathrm{GL}(2,\mathbb{R})$ which has the same central character and the same infinitesimal character as the finite-dimensional irreducible representation $\mathrm{Sym}^{n-1}(\mathbb{C}^2)$.

$$\sigma_n(\lambda) \stackrel{\mathrm{df}}{=} \sigma_n \otimes |\det|^{\lambda},$$

for each $\lambda \in \mathbb{C}$. More concretely, σ_n is induced from the neutral component:

$$\sigma_n = \mathrm{Ind}_{\mathrm{GL}(2,\mathbb{R})^+}^{\mathrm{GL}(2,\mathbb{R})}(\sigma_n^+),$$

where σ_n^+ is a certain representation of $\mathrm{GL}(2,\mathbb{R})^+$ on the Hilbert space of

$$f : \mathcal{H} \to \mathbb{C} \text{ holomorphic}, \quad \|f\|^2 = \int_{\mathcal{H}} |f(x+iy)|^2 y^{n-1} dx dy < \infty.$$

Here $\mathcal{H}$ denotes the upper half-plane in $\mathbb{C}$, and $\mathrm{GL}(2,\mathbb{R})^+$ acts by the formula

$$\sigma_n^+ \begin{pmatrix} a & c \\ b & d \end{pmatrix} f(z) = (ad-bc)^n (cz+d)^{-n-1} f(\frac{az+b}{cz+d}).$$

If instead of z we use $\bar{z}$ in the automorphy factor, this also defines a representation σ_n^- on the *anti*-holomorphic functions on $\mathcal{H}$. Then σ_n can be thought of as the direct sum $\sigma_n^+ \oplus \sigma_n^-$, where a non-trivial coset representative acts by reflection in the y-axis. Its Jacquet-Langlands correspondent σ_n^{JL} is simply $\mathrm{Sym}^{n-1}(\mathbb{C}^2)$ viewed as a representation of the Hamilton quaternions $\mathbb{H}^*$ embedded into $\mathrm{GL}(2,\mathbb{C})$ in the standard fashion. Note that σ_n is *not* unitary, unless $n = 1$. However, after a suitable twist it becomes unitary. Moreover,

$$\mathrm{Hom}_{\mathrm{GL}(2,\mathbb{R})^+}(\sigma_n^+(\frac{1-n}{2}), L^2_{\mathrm{cusp}}(\mathbb{R}_+^*\Gamma\backslash \mathrm{GL}(2,\mathbb{R})^+))$$

can be identified with the space of weight $n+1$ elliptic cusp forms for the discrete subgroup Γ. The weight $n+1$ is the Blattner parameter of σ_n, describing its minimal K-types. Up to isomorphism, σ_n is easily seen to be invariant under twisting by the sign character of $\mathbb{R}^*$. Consequently, σ_n is automorphically induced from a character on $\mathbb{C}^*$. More generally, its twist $\sigma_n(\lambda)$ is induced from

$$z \mapsto |z|^{2\lambda-1} z^n = |z|^{n-1+2\lambda}(z/\bar{z})^{\frac{n}{2}}.$$

We want to write down an L-parameter for $\sigma_n(\lambda)$. Thus, we let $W_{\mathbb{R}}$ denote the Weil group of $\mathbb{R}$, generated by $\mathbb{C}^*$ and an element j such that $j^2 = -1$ and $jz = \bar{z}j$ for all $z \in \mathbb{C}^*$. To $\sigma_n(\lambda)$ is associated a conjugacy class of homomorphisms

$$\phi_n(\lambda) : W_{\mathbb{R}} \to \mathrm{GL}(2,\mathbb{C})$$

with semisimple images. By the above remarks, a concrete representative is:

$$\phi_n(\lambda) : z \mapsto |z|^{n-1+2\lambda} \cdot \begin{pmatrix} (z/\bar{z})^{\frac{n}{2}} & \\ & (z/\bar{z})^{-\frac{n}{2}} \end{pmatrix}, \quad \phi_n(\lambda) : j \mapsto \begin{pmatrix} & 1 \\ (-1)^n & \end{pmatrix}.$$

We note that the image of $\phi_n(\lambda)$ is bounded precisely when $\sigma_n(\lambda)$ is unitary.

2.1.2 Discrete series for $\mathrm{GSp}(4,\mathbb{R})$

We parametrize the discrete series representations of $\mathrm{GSp}(4,\mathbb{R})$ in accordance with [Lau]. Throughout, we realize symplectic groups with respect to the form

$$J = \begin{pmatrix} & S \\ -S & \end{pmatrix}, \quad S = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}.$$

The similitude character is denoted by c. We take B to be the Borel subgroup consisting of upper triangular matrices. The maximal torus T is of the form

$$T = \{t = \begin{pmatrix} t_1 & & & \\ & t_2 & & \\ & & t_3 & \\ & & & t_4 \end{pmatrix} : c(t) = t_1 t_4 = t_2 t_3\}.$$

We identify its group of rational characters $X^*(T)$ with the set of triples of integers $\mu = \mu_0 \oplus (\mu_1, \mu_2)$, such that $\mu_1 + \mu_2 \equiv \mu_0 \pmod 2$, using the recipe:

$$t^\mu \overset{\mathrm{df}}{=} t_1^{\mu_1} t_2^{\mu_2} c(t)^{\frac{\mu_0 - \mu_1 - \mu_2}{2}}.$$

Its restriction to the center $\mathbb{G}_m$ takes $a \mapsto a^{\mu_0}$. Inside $X^*(T)$ we have the cone of B-dominant weights $X^*(T)^+$ consisting of all tuples μ such that $\mu_1 \geq \mu_2 \geq 0$. By a fundamental result of Chevalley, the finite-dimensional irreducible algebraic representations are classified by their highest weights. For a B-dominant weight μ as above, we let V_μ be the corresponding algebraic representation of $\mathrm{GSp}(4)$. Its central character is given by μ_0 as described above. To describe the infinitesimal character of V_μ, we consider half the sum of B-positive roots:

$$\delta \overset{\mathrm{df}}{=} 0 \oplus (2, 1).$$

The Harish-Chandra isomorphism identifies the center of the universal enveloping algebra, $Z(\mathfrak{g})$, with the invariant symmetric algebra $\mathrm{Sym}(\mathfrak{t}_\mathbb{C})^W$. Under this isomorphism, the aforementioned infinitesimal character corresponds to

$$\nu \overset{\mathrm{df}}{=} \mu + \delta = \mu_0 \oplus (\nu_1, \nu_2) = \mu_0 \oplus (\mu_1 + 2, \mu_2 + 1).$$

Up to infinitesimal equivalence, there are precisely *two* essentially discrete series representations of $\mathrm{GSp}(4,\mathbb{R})$ with the same central character and the same infinitesimal character as V_μ. Together, they form an L-packet,

$$\{\pi_\mu^W, \pi_\mu^H\}.$$

Here π_μ^W is the unique *generic* member, that is, it has a Whittaker model. The other member π_μ^H is *holomorphic*, and does not have a Whittaker model. They both have central character $a \mapsto a^{\mu_0}$ for real nonzero a. Another way to distinguish the two representations, is to look at their $(\mathfrak{g}, K)$-cohomology: The generic member π_μ^W has cohomology of Hodge type $(2,1)$ and $(1,2)$, whereas π_μ^H contributes cohomology of Hodge type $(3,0)$ and $(0,3)$. For example,

$$H^{3,0}(\mathfrak{g},K;\pi_\mu^H\otimes V_\mu^*)\simeq H^{0,3}(\mathfrak{g},K;\pi_\mu^H\otimes V_\mu^*)\simeq\mathbb{C},$$

and similarly for π_μ^W. We have consistently used the Harish-Chandra parameter ν. Other authors prefer the Blattner parameter, because of its connection to the weights of Siegel modular forms. In our case, the relation is quite simple:

$$\underline{k}=(k_1,k_2),\quad k_1=\nu_1+1=\mu_1+3,\quad k_2=\nu_2+2=\mu_2+3.$$

See Theorem 12.21 in [Kn] for example. A word of caution: It is really only fair to call $\underline{k}$ the Blattner parameter in the holomorphic case. In the generic case, it does not give the highest weight of the minimal K-type. The restriction of π_μ^H to the neutral component $\mathrm{GSp}(4,\mathbb{R})^+$, consisting of elements with positive similitude, decomposes as a direct sum of a holomorphic part π_μ^{H+} and a dual anti-holomorphic part π_μ^{H-}. If we assume $\mu_0=0$, so that these are unitary,

$$\mathrm{Hom}_{\mathrm{GSp}(4,\mathbb{R})^+}(\pi_\mu^{H+},L^2_{\mathrm{cusp}}(\mathbb{R}_+^*\Gamma\backslash\mathrm{GSp}(4,\mathbb{R})^+))$$

can be identified with cuspidal Siegel modular forms of weight $\underline{k}$ for the discrete subgroup Γ. The minimal K-type of π_μ^{H+}, where K is isomorphic to $\mathrm{U}(2)$, is

$$\mathrm{Sym}^{k_1-k_2}(\mathbb{C}^2)\otimes\det{}^{k_2}.$$

This is the algebraic representation of $\mathrm{GL}(2,\mathbb{C})$ with highest weight $t_1^{k_1}t_2^{k_2}$. Next, we wish to explain how π_μ^W and π_μ^H can be described explicitly as certain theta lifts: Up to equivalence, there are precisely two 4-dimensional quadratic spaces over $\mathbb{R}$ of discriminant one. Namely, the anisotropic space $V_{4,0}$ and the split space $V_{2,2}$. The latter can be realized as $\mathrm{M}(2,\mathbb{R})$ equipped with the determinant. The former can be taken to be $\mathbb{H}$ endowed with the reduced norm. In particular,

$$\mathrm{GSO}(2,2)=(\mathrm{GL}(2,\mathbb{R})\times\mathrm{GL}(2,\mathbb{R}))/\mathbb{R}^*,\quad \mathrm{GSO}(4,0)=(\mathbb{H}^*\times\mathbb{H}^*)/\mathbb{R}^*.$$

Here $\mathbb{R}^*$ is embedded in the centers by taking a to the element (a,a^{-1}). Thus irreducible representations of $\mathrm{GSO}(2,2)$ correspond to pairs of irreducible representations of $\mathrm{GL}(2,\mathbb{R})$ having the same central character. Similarly for $\mathrm{GSO}(4,0)$. Now suppose σ and σ' are irreducible representations of $\mathrm{GL}(2,\mathbb{R})$ with the same central character. We say that the representation $\sigma\otimes\sigma'$ is *regular* if $\sigma\neq\sigma'$. The induced representation of the whole similitude group $\mathrm{GO}(2,2)$ then remains irreducible, and we denote it by $(\sigma\otimes\sigma')^+$ following the notation of [Rob]. On the other hand, in the *invariant* case where $\sigma=\sigma'$, there are exactly two extensions of $\sigma\otimes\sigma$ to a representation of $\mathrm{GO}(2,2)$. By Theorem 6.8 in [Rob], precisely one of these extensions participates in the theta correspondence with $\mathrm{GSp}(4,\mathbb{R})$. It is again denoted by $(\sigma\otimes\sigma)^+$. The analogous results hold in the anisotropic case. Now, the following two identities can be found in several places in the literature. See [Moe] for example, or Proposition 4.3.1 in [HK]:

$$\pi_\mu^W=\theta((\sigma_{\nu_1+\nu_2}(\frac{1}{2}(\mu_0-\nu_1-\nu_2+1))\otimes\sigma_{\nu_1-\nu_2}(\frac{1}{2}(\mu_0-\nu_1+\nu_2+1)))^+),$$

and

$$\pi_\mu^H=\theta((\sigma^{\mathrm{JL}}_{\nu_1+\nu_2}(\frac{1}{2}(\mu_0-\nu_1-\nu_2+1))\otimes\sigma^{\mathrm{JL}}_{\nu_1-\nu_2}(\frac{1}{2}(\mu_0-\nu_1+\nu_2+1)))^+).$$

Here the equalities signify infinitesimal equivalence. Since we are dealing with theta correspondence for *similitude* groups, it is unnecessary to specify an additive character. As a result, we can exhibit a parameter for the μ-packet above:

$$\phi_\mu: z\mapsto |z|^{\mu_0}\cdot\begin{pmatrix}(z/\bar{z})^{\frac{\nu_1+\nu_2}{2}} & & & \\ & (z/\bar{z})^{\frac{\nu_1-\nu_2}{2}} & & \\ & & (z/\bar{z})^{-\frac{\nu_1-\nu_2}{2}} & \\ & & & (z/\bar{z})^{-\frac{\nu_1+\nu_2}{2}}\end{pmatrix},$$

and

$$\phi_\mu: j\mapsto\begin{pmatrix} & & & 1\\ & & 1 & \\ & (-1)^{\mu_0+1} & & \\ (-1)^{\mu_0+1} & & & \end{pmatrix}.$$

Visibly, ϕ_μ maps into the dual of the elliptic endoscopic group, consisting of

$$\begin{pmatrix}a & & & b\\ & e & f & \\ & g & h & \\ c & & & d\end{pmatrix}=\begin{pmatrix}1 & & & \\ & & 1 & \\ & & & 1\\ & 1 & & \end{pmatrix}\begin{pmatrix}a & b & & \\ c & d & & \\ & & e & f\\ & & g & h\end{pmatrix}\begin{pmatrix}1 & & & \\ & & 1 & \\ & & & 1\\ & 1 & & \end{pmatrix}^{-1}$$

such that $ad-bc$ equals $eh-fg$. Furthermore, the restriction of $\phi_\mu\otimes|\cdot|^{-3}$ to $\mathbb{C}^*$ is a direct sum of *distinct* characters of the form $z\mapsto z^p\bar{z}^q$ for two *integers* p and q such that $p+q=\mu_0-3$. They come in pairs: If the type (p,q) occurs, so does (q,p). We say that π_μ^W and π_μ^H are regular algebraic (up to a twist).

2.1.3 THE LANGLANDS CLASSIFICATION FOR $\mathrm{GL}(4,\mathbb{R})$

The Langlands classification for $\mathrm{GL}(4,\mathbb{R})$ describes all its irreducible admissible representations up to infinitesimal equivalence. The building blocks are the essentially discrete series $\sigma_n(\lambda)$, and the characters $\mathrm{sgn}^n(\lambda)$ of the multiplicative group $\mathbb{R}^*$. The representations of $\mathrm{GL}(4,\mathbb{R})$ are then constructed by parabolic induction. For example, start out with the representations $\sigma_n(\lambda)$ and $\sigma_{n'}(\lambda')$.

We view their tensor product as a representation of the parabolic associated with the partition $(2,2)$, by making it trivial on the unipotent radical. Consider

$$\mathrm{Ind}_{P_{(2,2)}}^{\mathrm{GL}(4,\mathbb{R})}(\sigma_n(\lambda)\otimes\sigma_{n'}(\lambda')),$$

where we use *normalized* induction. Consequently, this is unitary when $\sigma_n(\lambda)$ and $\sigma_{n'}(\lambda')$ are both unitary. By interchanging their roles, we may assume that

$$\mathrm{Re}(\lambda)\geq\mathrm{Re}(\lambda').$$

In this case, the induced representation has a unique irreducible quotient. We denote it by $\sigma_n(\lambda)\boxplus\sigma_{n'}(\lambda')$ and call it the *isobaric* sum. Its L-parameter is

$$\phi=\phi_n(\lambda)\oplus\phi_{n'}(\lambda'):W_{\mathbb{R}}\to\mathrm{GL}(4,\mathbb{C}).$$

We want to know when it descends to a parameter for $\mathrm{GSp}(4,\mathbb{R})$. First, in the case where $n=n'$, it maps into the Levi subgroup of the Siegel parabolic:

$$P=\{\begin{pmatrix}A & \\ & c\cdot{}^{\tau}A^{-1}\end{pmatrix}\begin{pmatrix}1 & & x & y\\ & 1 & z & x\\ & & 1 & \\ & & & 1\end{pmatrix}\}.$$

Here τ is transposition with respect to the *skew* diagonal. This means the packet for $\mathrm{GSp}(4,\mathbb{R})$ should be obtained by induction from the Klingen parabolic,

$$Q=\{\begin{pmatrix}t & & \\ & A & \\ & & t^{-1}\det(A)\end{pmatrix}\begin{pmatrix}1 & z & & \\ & 1 & & \\ & & 1 & -z\\ & & & 1\end{pmatrix}\begin{pmatrix}1 & & x & y\\ & 1 & & x\\ & & 1 & \\ & & & 1\end{pmatrix}\}.$$

To be more precise, consider the following (unitarily) induced representation:

$$\mathrm{Ind}_{Q}^{\mathrm{GSp}(4,\mathbb{R})}(\sigma_n(\lambda')\otimes|\cdot|^{2\lambda-2\lambda'}).$$

When $\mathrm{Re}(\lambda)$ is *strictly* greater than $\mathrm{Re}(\lambda')$ it has a unique irreducible quotient. At the other extreme, when $\lambda=\lambda'$ it decomposes into a direct sum of two *limits* of discrete series. Secondly, in the case where $n\neq n'$ we try to conjugate ϕ into the dual of the elliptic endoscopic group. The determinant condition becomes:

$$\lambda-\lambda'=\frac{1}{2}(n'-n)\in\mathbb{Z}_{+}. \tag{1}$$

If this is satisfied, the isobaric sum descends to a packet for $\mathrm{GSp}(4,\mathbb{R})$, whose members can be constructed by theta correspondence as discussed above:

$$\{\pi_{\mu}^{W},\pi_{\mu}^{H}\},\quad \mu_0=n-1+2\lambda,\quad \nu_1=\frac{1}{2}(n'+n),\quad \nu_2=\frac{1}{2}(n'-n).$$

2.2 The non-archimedean case

2.2.1 The local Langlands correspondence for GL(n)

We will quickly review the parametrization of the irreducible admissible representations of $\mathrm{GL}(n,F)$, up to isomorphism, where F is a finite extension of $\mathbb{Q}_p$. We will suppress F and denote this set by $\Pi(\mathrm{GL}(n))$. This parametrization was originally conjectured by Langlands, for any connected reductive group, and recently proved for $\mathrm{GL}(n)$ in [HT] and [Hen] by two different methods. We let W_F be the Weil group of F. That is, the dense subgroup of the Galois group acting as integral powers of Frobenius on the residue field. It gets a topology by decreeing that the inertia group I_F is open. From local class field theory,

$$F^* \xrightarrow{\sim} W_F^{\mathrm{ab}}.$$

Here the isomorphism is normalized such that uniformizers correspond to lifts of the geometric Frobenius. It is used tacitly to identify characters of F^* with characters of W_F. For arbitrary n, we consider the set $\Phi(\mathrm{GL}(n))$ consisting of conjugacy classes of continuous semisimple n-dimensional representations

$$\phi : W_F' = W_F \times \mathrm{SL}(2,\mathbb{C}) \to \mathrm{GL}(n,\mathbb{C}).$$

The group W_F' is sometimes called the Weil-Deligne group. The local Langlands correspondence is then a canonical collection of bijections rec_n, one for each n,

$$\mathrm{rec}_n : \Pi(\mathrm{GL}(n)) \xrightarrow{1:1} \Phi(\mathrm{GL}(n))$$

associating an L-parameter ϕ_π to a representation π. It satisfies a number of natural properties, which in fact determine the collection uniquely. Namely,

- The bijection rec_1 is given by local class field theory as above.
- For any two $\pi \in \Pi(\mathrm{GL}(n))$ and $\sigma \in \Pi(\mathrm{GL}(r))$, we have equalities

$$\begin{cases} L(s,\pi\times\sigma) = L(s,\phi_\pi\otimes\phi_\sigma), \\ \epsilon(s,\pi\times\sigma,\psi) = \epsilon(s,\phi_\pi\otimes\phi_\sigma,\psi). \end{cases}$$

- The L-parameter of $\pi\otimes\chi\circ\det$ equals $\phi_\pi\otimes\chi$, for any character χ.
- For any π as above, $\det(\phi_\pi)$ corresponds to its central character ω_π.
- For any π as above, $\mathrm{rec}_n(\pi^\vee)$ is the contragredient of $\mathrm{rec}_n(\pi)$.

Here ψ is a non-trivial character of F, used to define the ϵ-factors. The collection rec_n does not depend on it. The L and ϵ-factors on the left-hand side are those from [JPS]: They are first defined for generic representations, such as supercuspidals, and then one extends the definition to all representations using the Langlands classification. For the explicit formulas, see [Kud] or [Wed].

For the right-hand side, the definition of the L and ϵ-factors can be found in [Tat]: The L-factors are given fairly explicitly, whereas the ϵ-factors are defined very implicitly. One only has an abstract characterization due to Deligne and Langlands. For a good review of these definitions, we again refer to [Wed]. It is useful to instead consider the (Frobenius semisimple) Weil-Deligne representation of W_F associated with a parameter ϕ as above. This is a pair (r, N) consisting of a semisimple representation r of W_F, and an operator N satisfying the equation

$$r(w) \circ N \circ r(w)^{-1} = |w|_F \cdot N$$

for all $w \in W_F$. This N is called the monodromy operator, and it is automatically nilpotent. The correspondence relies on the Jacobson-Morozov theorem:

$$r(w) = \phi(w, \begin{pmatrix} |w|_F^{\frac{1}{2}} & \\ & |w|_F^{-\frac{1}{2}} \end{pmatrix}), \quad \exp(N) = \phi(1, \begin{pmatrix} 1 & 1 \\ & 1 \end{pmatrix}).$$

The local Langlands correspondence rec_n satisfies a number of additional natural properties, expected to hold more generally, of which we mention only a few:

- π is supercuspidal $\Leftrightarrow$ ϕ_π is irreducible (and the monodromy is trivial).
- π is essentially discrete series $\Leftrightarrow$ ϕ_π does *not* map into a proper Levi.
- π is essentially tempered $\Leftrightarrow$ $\phi_\pi|_{W_F}$ has *bounded* image in $\mathrm{GL}_n(\mathbb{C})$.
- π is generic $\Leftrightarrow$ the adjoint L-factor $L(s, \mathrm{Ad} \circ \phi_\pi)$ has *no* pole at $s = 1$.

Here Ad denotes the adjoint representation of $\mathrm{GL}_n(\mathbb{C})$ on its Lie algebra $\mathfrak{gl}_n(\mathbb{C})$.

2.2.2 The local Langlands correspondence for GSp(4)

For GSp(4), the presence of endoscopy makes the parametrization of $\Pi(\mathrm{GSp}(4))$ more complicated. It is partitioned into finite subsets L_ϕ, called L-packets, each associated with a parameter ϕ as above mapping into the subgroup $\mathrm{GSp}(4, \mathbb{C})$. We use the notation $\Phi(\mathrm{GSp}(4))$ for the set of $\mathrm{GSp}(4, \mathbb{C})$-conjugacy classes of such ϕ. The first attempt to define these L-packets, when p is *odd*, is the paper [Vig]. The crucial case is when ϕ does not map into a proper Levi subgroup. In this case, Vigneras defined certain subsets L_ϕ by theta lifting from various forms of GO(4). However, she did not prove that these L_ϕ *exhaust* all of $\Pi(\mathrm{GSp}(4))$. The work of Vigneras was later refined, so as to include the case $p = 2$, in the paper [Ro2]. More recently, Gan and Takeda [GT] were able to prove the exhaustion, for all primes p. To do that, they used work of Muic-Savin, Kudla-Rallis, and Henniart. The main theorem of [GT] gives a finite-to-one surjection

$$L : \Pi(\mathrm{GSp}(4)) \twoheadrightarrow \Phi(\mathrm{GSp}(4)),$$

attaching an L-parameter ϕ_π to a representation π, and having the properties:

- π is essentially discrete series $\Leftrightarrow$ ϕ_π does *not* map into a proper Levi.
- For any generic *or* non-supercuspidal $\pi \in \Pi(\mathrm{GSp}(4))$, and $\sigma \in \Pi(\mathrm{GL}(r))$,

$$\begin{cases} \gamma(s, \pi \times \sigma, \psi) = \gamma(s, \phi_\pi \otimes \phi_\sigma, \psi), \\ L(s, \pi \times \sigma) = L(s, \phi_\pi \otimes \phi_\sigma), \\ \epsilon(s, \pi \times \sigma, \psi) = \epsilon(s, \phi_\pi \otimes \phi_\sigma, \psi). \end{cases}$$

- The L-parameter of $\pi \otimes \chi \circ c$ equals $\phi_\pi \otimes \chi$, for any character χ.
- For any π as above, $c(\phi_\pi)$ corresponds to its central character ω_π.

In the generic case, the invariants occurring on the left-hand side of the second condition are those from [Sha]. The definition can be extended to non-generic non-supercuspidals, using the Langlands classification. See page 13 in [GT]. For non-generic supercuspidals, L satisfies an additional technical identity, which we will not state here. It expresses a certain Plancherel measure as a product of four γ-factors. One has to include this last property to ensure the *uniqueness* of L, as long as a satisfying theory of γ-factors is absent in this setup. For completeness, let us mention a few extra properties of the map L: For a given parameter ϕ, the elements of the fiber L_ϕ correspond to characters of the group

$$A_\phi = \pi_0(Z_{\mathrm{GSp}(4,\mathbb{C})}(\mathrm{im}\phi)/\mathbb{C}^*) = \begin{cases} \mathbb{Z}/2\mathbb{Z}, \\ 0. \end{cases}$$

Moreover, an L-packet L_ϕ contains a generic member exactly when $L(s, \mathrm{Ad}\circ\phi)$ has no pole at $s = 1$. If in addition $\phi|_{W_F}$ has bounded image, the members of L_ϕ are all essentially tempered, and the generic member is unique. It is indexed by the trivial character of A_ϕ. Next, we wish to at least give some idea of how the reciprocity map L is constructed in [GT]: The key is to make use of theta liftings from various orthogonal similitude groups. In analogy with the archimedean case, there are two 4-dimensional quadratic spaces over F of discriminant one. We abuse notation slightly, and continue to denote the anisotropic space by $V_{4,0}$ and the split space by $V_{2,2}$. They can be realized as D equipped with the reduced norm, where D is a possibly split quaternion algebra over F. Again,

$$\mathrm{GSO}(2,2) = (\mathrm{GL}(2,F) \times \mathrm{GL}(2,F))/F^*, \quad \mathrm{GSO}(4,0) = (D^* \times D^*)/F^*,$$

as previously, where D is here the *division* quaternion algebra. Furthermore, one looks at the 6-dimensional quadratic space $D \oplus V_{1,1}$. When D is split, this is simply $V_{3,3}$. There is then a natural isomorphism, as given on page 9 in [GT],

$$\mathrm{GSO}(3,3) = (\mathrm{GL}(4,F) \times F^*)/\{(a \cdot I, a^{-2}) : a \in F^*\}.$$

Now, start with an irreducible representation π of $\mathrm{GSp}(4,F)$. By Theorem 5.3 in [GT], which relies on the work [KR] of Kudla and Rallis on the conservation conjecture, it follows that there are two possible *mutually exclusive* scenarios:

1. π participates in the theta correspondence with $\mathrm{GSO}(4,0)$,
2. π participates in the theta correspondence with $\mathrm{GSO}(3,3)$.

In the *first* case, one has two essentially discrete series representations σ and σ' of $\mathrm{GL}(2,F)$ having the same central character, such that π is the theta lift

$$\pi = \theta((\sigma^{\mathrm{JL}} \otimes \sigma'^{\mathrm{JL}})^+) = \theta((\sigma'^{\mathrm{JL}} \otimes \sigma^{\mathrm{JL}})^+).$$

By the local Langlands correspondence for $\mathrm{GL}(2)$, we have associated parameters ϕ_σ and $\phi_{\sigma'}$ with equal determinants. We then conjugate their sum $\phi_\sigma \oplus \phi_{\sigma'}$ into the dual of the elliptic endoscopic group as in the archimedean case,

$$\phi_\pi = \phi_\sigma \oplus \phi_{\sigma'} : W_F' \to \mathrm{GL}(2,\mathbb{C}) \times_{\mathbb{C}^*} \mathrm{GL}(2,\mathbb{C}) \subset \mathrm{GSp}(4,\mathbb{C}).$$

In the *second* case, we write $\theta(\pi)$ as a tensor product $\Pi \otimes \omega_\pi$ for an irreducible representation Π of $\mathrm{GL}(4,F)$. The local Langlands correspondence for $\mathrm{GL}(4)$ yields a parameter ϕ_Π. We need to know that it maps into $\mathrm{GSp}(4,\mathbb{C})$ after conjugation. When π is a *discrete* series, this follows from a result of Muic and Savin [MS], stated as Theorem 5.4 in [GT]: Indeed, the exterior square L-factor

$$L(s, \Pi, \wedge^2 \otimes \omega_\pi^{-1})$$

has a pole at $s = 0$. When π is *not* a discrete series, Gan and Takeda compute $\theta(\pi)$ explicitly, using standard techniques developed by Kudla. For a summary, we refer to Table 2 on page 51 in their paper [GT]. It follows by *inspection* that ϕ_Π can be conjugated into a Levi subgroup of $\mathrm{GSp}(4,\mathbb{C})$. Their computation works even for $p = 2$, and hence completes the *exercise* of Waldspurger [Wal]. Finally, in Proposition 11.1 of [GT], it is shown by a global argument that the above construction is consistent with that of Vigneras and Roberts.

2.3 The globally generic case

In the global situation, functoriality predicts that one should be able to transfer automorphic representations from $\mathrm{GSp}(4)$ to $\mathrm{GL}(4)$. It is widely believed that this should eventually follow by using trace formula techniques. See [Art] for a discussion on this approach. In the *globally generic* case, it has been known for some time that one can obtain (weak) lifts using theta series. This was first announced by Jacquet, Piatetski-Shapiro and Shalika, but to the best of our knowledge they never wrote it up. However, many of the details are to be found in [Sou]. Moreover, there is an alternative proof in [AS] relying on the converse theorem. In this section, we wish to quote a recent refinement of the above transfer, due to Gan and Takeda [GT]. First, for completeness, let us recall the notion of being globally generic: Consider the upper-triangular Borel subgroup

$$B = \{\begin{pmatrix} s & & & \\ & t & & \\ & & ct^{-1} & \\ & & & cs^{-1}\end{pmatrix}\begin{pmatrix} 1 & u & & \\ & 1 & & \\ & & 1 & -u \\ & & & 1\end{pmatrix}\begin{pmatrix} 1 & & x & y \\ & 1 & z & x \\ & & 1 & \\ & & & 1\end{pmatrix}\}.$$

We let N denote its unipotent radical. Now let F be a number field, and pick a non-trivial character ψ of $\mathbb{A}_F$ trivial on F. By looking at $\psi(u+z)$ we can view it as an automorphic character of N. An automorphic representation π of GSp(4) over F is then said to be globally generic if the Whittaker functional

$$f \mapsto \int_{N(F)\backslash N(\mathbb{A}_F)} f(n)\psi^{-1}(n)dn, \quad f \in \pi,$$

is not identically zero. This notion does not depend on ψ. As a consequence of the theta series approach we are about to discuss, Soudry proved the strong multiplicity one property in [Sou] for globally generic cusp forms π on GSp(4). As mentioned above, the exterior square $\wedge^2$ defines an isogeny between the groups GL(4) and GSO(3,3). Thus, we need the global theta correspondence for *similitude* groups. For this, we refer to section 5 of [HK], noting that the normalization there differs slightly from [GT]. We will quickly review the main features of the definition: The Weil representation ω_ψ extends naturally to

$$R = \{(g,h) \in \mathrm{GSp}(4) \times \mathrm{GO}(3,3) : c(g) \cdot c(h) = 1\}.$$

Then, a Schwartz-Bruhat function φ defines a theta kernel θ_φ on R by the usual formula. The theta series lifting of a form f in π is hence given by the integral

$$\theta_\varphi(f)(h) = \int_{\mathrm{Sp}(4,F)\backslash \mathrm{Sp}(4,\mathbb{A}_F)} \theta_\varphi(gg_h, h) f(gg_h)dg,$$

where g_h is any element with inverse similitude $c(h)$. The space spanned by all such theta series $\theta_\varphi(f)$ constitute an automorphic representation of GO(3,3), which we will denote by $\theta(\pi)$. It is independent of ψ. By Proposition 1.2 in [Sou], it is nonzero precisely when π is globally generic. In fact, one can express the Whittaker functional for $\theta(\pi)$ in terms of that for π given above. In particular, $\theta(\pi)$ is always generic, even though it may not be cuspidal. From now on, we will only view $\theta(\pi)$ as a representation of the subgroup GSO(3,3). As such, it remains irreducible. See Lemma 3.1 in [GT] for example. In turn, via the identification $\wedge^2$ we view $\theta(\pi)$ as a representation $\Pi \otimes \omega_\pi$. We then have:

Theorem 1. *The global theta lifting $\pi \mapsto \theta(\pi) = \Pi \otimes \omega_\pi$ defines an injection from the set of globally generic cuspidal automorphic representations π of GSp(4) to the set of generic automorphic representations Π of GL(4) with central character $\omega_\Pi = \omega_\pi^2$. Moreover, this lifting has the following properties:*

- $\Pi \simeq \Pi^\vee \otimes \omega_\pi$.
- *It is a* strong *lift, that is, $\phi_{\Pi_v} = \phi_{\pi_v}$ for all places v.*
- *The image of the lifting consists* precisely *of those Π satisfying:*
    1. *Π is cuspidal and $L^S(s, \Pi, \wedge^2 \otimes \omega_\pi^{-1})$ has a pole at $s=1$,* or

2. $\Pi = \sigma \boxplus \sigma'$ *for cuspidal* $\sigma \neq \sigma'$ *on* $GL(2)$ *with central character* ω_π.

In the latter case, π *is the theta lift of the cusp form* $\sigma \otimes \sigma'$ *on* $GSO(2,2)$.

Proof. See section 13 in [GT]. □

The refinements, due to Gan and Takeda, are primarily: The characterization of the image, and the fact that the global lift is compatible with the local Langlands correspondence at all (finite) places. The result that the lift is *strong*, in this sense, essentially follows from the construction of the local reciprocity map. However, locally one has to check that ϕ_Π is equivalent to $\phi_\sigma \oplus \phi_{\sigma'}$, when π is the theta lift of *any* $\sigma \otimes \sigma'$ on $\mathrm{GSO}(2,2)$. This is the content of Corollary 12.13 in [GT]. It is a result of their explicit determination of the theta correspondence.

3 Base change to a CM extension

In this section we will construct representations, for which the results from [HT] on Galois representations apply. For that purpose, we will fix an arbitrary CM (quadratic) extension E/F, and an arbitrary Hecke character χ of E with the property:

$$\chi|_{\mathbb{A}_F^*} = \omega_\pi^{-1}.$$

Since ω_{π_v} is of the form $a \mapsto a^{-w}$ at each infinite place v, it follows that every such χ is automatically algebraic. For all but finitely many E, the global base change Π_E, to be defined below, is *cuspidal*. In fact, we will choose a suitable quadratic CM extension E of F such that v_0 is totally split in E, and a suitable Hecke character χ of E. The suitability refers to the fact that the Arthur-Clozel base change Π_E will be cuspidal, and that its twist by χ will be conjugate self-dual,

$$\Pi_E(\chi)^\theta \simeq \Pi_E(\chi)^\vee.$$

Furthermore, $\Pi_E(\chi)$ is regular algebraic of weight zero, and we can arrange for it to have at least one square integrable component, by imposing the condition that E splits completely at v_0. Hence Theorem C in [HT] applies. In this section, we briefly review results of Arthur and Clozel on base change for $\mathrm{GL}(n)$, and discuss the compatibility with the local Langlands correspondence.

3.1 Local base change

Now that the p-adic local Langlands correspondence is available for $\mathrm{GL}(n)$, due to the works of Harris-Taylor and Henniart, base change makes sense for an arbitrary finite extension of local fields E/F. Indeed, a representation Π_E of $\mathrm{GL}(n,E)$ is the base change of a representation Π of $\mathrm{GL}(n,F)$ precisely when

$$\phi_{\Pi_E} = \phi_\Pi|_{W_E'}.$$

However, eventually we will use results from [AC]. At the time this book was written, one had to resort to a harmonic analytic definition of base change which we will review below. Fortunately, the compatibility of the two definitions has been checked by other authors. We will give precise references later. The latter definition only works for a cyclic extension E/F. For simplicity, we take it to be quadratic, and let θ be the non-trivial element in its Galois group. By lemma 1.1 in [AC], the norm map on $GL(n,E)$, taking $\gamma \mapsto \gamma\gamma^\theta$, defines an injection

$$\mathcal{N} : \{\theta\text{-conjugacy classes in } \mathrm{GL}(n,E)\} \hookrightarrow \{\text{conjugacy classes in } \mathrm{GL}(n,F)\}.$$

This is used to define transfer of orbital integrals: Two compactly supported smooth functions f and f_E are said to have matching orbital integrals when

$$O_\gamma(f) = \begin{cases} TO_{\delta\theta}(f_E), & \gamma = \mathcal{N}\delta, \\ 0, & \gamma \text{ is } \textit{not} \text{ a norm.} \end{cases}$$

For the definitions of the integrals involved here, we refer to page 15 in [AC]. It is the content of Proposition 3.1 in [AC] that any f_E has a matching function f. The fundamental lemma in this case is Theorem 4.5 in [AC]. We can now state Shintani's definition of local base change, following Definition 6.1 in [AC]: Let Π and Π_E be irreducible admissible representations of $\mathrm{GL}(n,F)$ and $\mathrm{GL}(n,E)$ respectively, and assume that Π_E^θ is isomorphic to Π_E. Let I_θ be an intertwining operator between these, normalized such that I_θ^2 is the identity. This determines I_θ up to a sign. We then say that Π_E is a base change of Π if and only if

$$\mathrm{tr}(\Pi_E(f_E) \circ I_\theta) = c \cdot \mathrm{tr}\Pi(f)$$

for all matching functions f and f_E as above. The non-zero constant c depends only on the choice of measures, and of I_θ. By Theorem 6.2 in [AC] local base change makes sense for tempered representations. Using the Langlands classification, the lift then extends to all representations. For this, see the discussion on page 59 in [AC]. Since Shintani's definition is employed in [AC], we will need:

Theorem 2. *Shintani's harmonic analytic definition of the local cyclic base change lifting is compatible with the local Langlands correspondence for GL(n).*

Proof. In the non-archimedean case, this is part 5 of Lemma VII.2.6 on page 237 in [HT]. The archimedean case was settled, in general, by Clozel [Clo]. □

As an example in the archimedean case, let us base change $\sigma_n(\lambda) \boxplus \sigma_{n'}(\lambda')$ to $\mathrm{GL}(4,\mathbb{C})$. For simplicity, we will stick to the case of interest in this paper where it descends to a discrete series L-packet for $\mathrm{GSp}(4,\mathbb{R})$. That is, we assume (1).

$$-w \overset{\mathrm{df}}{=} n - 1 + 2\lambda = n' - 1 + 2\lambda'$$

Following [Kna] we let $[z]$ denote $\frac{z}{|z|}$. Then the unitarily induced representation

$$\mathrm{Ind}_B^{\mathrm{GL}(4,\mathbb{C})}([\cdot]^n \otimes [\cdot]^{-n} \otimes [\cdot]^{n'} \otimes [\cdot]^{-n'}) \otimes |\det|^{-w}$$

has a unique irreducible quotient. This is the base change we are looking for. The Langlands correspondence for $\mathrm{GL}(n,\mathbb{C})$, which is much simpler than the real case, was first studied by Zelobenko and Naimark. A good reference for their results is the expository paper [Kna]. In the non-archimedean case,

$$\mathrm{St}_{\mathrm{GL}(4)}(\chi)_E = \mathrm{St}_{\mathrm{GL}(4)}(\chi_E), \quad \chi_E = \chi \circ N_{E/F}.$$

However, the generalized Steinberg representation $\mathrm{St}(\tau)$ may *not* base change to a discrete series. Indeed, if $\omega_{E/F}$ denotes the associated quadratic character,

$$\mathrm{St}(\tau)_E = \begin{cases} \mathrm{St}(\tau_E) \\ \mathrm{St}_{\mathrm{GL}(2)}(\psi) \boxplus \mathrm{St}_{\mathrm{GL}(2)}(\psi^\theta) \end{cases} \quad \text{when} \quad \begin{cases} \tau \neq \tau \otimes \omega_{E/F} \\ \tau = \tau \otimes \omega_{E/F}. \end{cases}$$

Here $\psi \neq \psi^\theta$ is a certain character of E^*, with automorphic induction τ.

3.2 Global base change

We now let E/F denote an arbitrary CM extension of the totally real field F. Thus, the extension E/F is quadratic, and E is totally imaginary. We let θ be the non-trivial element in the Galois group. Let Π and Π_E be automorphic representations of $\mathrm{GL}(n,\mathbb{A}_F)$ and $\mathrm{GL}(n,\mathbb{A}_E)$ respectively. We will assume Π_E is invariant under θ. Then, we say that Π_E is a *strong* base change lift of Π if

$$\Pi_{E,w} = \Pi_{v,E_w}$$

for *all* places $w|v$. Here, the right-hand side is the local base change of Π_v to $\mathrm{GL}(n,E_w)$. When v is *split* in E, this lift is naturally identified with Π_v. By comparing trace formulas for $\mathrm{GL}(n)$, no stabilization required, Arthur and Clozel proved that such lifts always exist. More precisely, we have the following:

Theorem 3. *There is a unique* strong *base change lift* $\Pi \mapsto \Pi_E$ *between isobaric automorphic representations on* $GL(n,\mathbb{A}_F)$ *and* $GL(n,\mathbb{A}_E)$*, satisfying:*

- $\omega_{\Pi_E} = \omega_\Pi \circ N_{E/F}$.
- *The image of the lifting consists* precisely *of the θ-invariant* Π_E.
- *If* Π *is cuspidal,* Π_E *is cuspidal if and only if* $\Pi \neq \Pi \otimes \omega_{E/F}$.

Proof. This is essentially Theorem 4.2 combined with Theorem 5.1 in [AC]. Arthur and Clozel makes the assumption that Π is *induced* from *cuspidal*. This is now superfluous; the residual spectrum of $\mathrm{GL}(n)$ is understood by [MW]. □

Note that, if Π is cuspidal, Π_E is cuspidal for all but finitely many CM extensions E. Indeed, the self-twist condition is satisfied if the discriminant of E does not divide the conductor of Π. The theory of base change goes hand-in-hand with *automorphic induction*, which is a strong lift from isobaric automorphic representations of $\mathrm{GL}(n,\mathbb{A}_E)$ to those of $\mathrm{GL}(2n,\mathbb{A}_F)$ compatible with the rec_n,

$$\pi \mapsto I_E^F(\pi), \quad \phi_{I_E^F(\pi)_v} = \mathrm{Ind}_{E_w}^{F_v}(\phi_{\pi_w}),$$

for all $w|v$. Again, this is due to Arthur and Clozel in much greater generality. See Theorem 6.2 in [AC]. For the compatibility with rec_n at the ramified places, we again refer to Lemma VII.2.6 in [HT]. In analogy with the above, we have the following result, which is not needed for the proof of the main theorem, but we include it for future use:

Theorem 4. *There is a* STRONG *automorphic induction lift* $\pi \mapsto I_E^F(\pi)$ *between isobaric automorphic representations on* $GL(n, \mathbb{A}_E)$ *and* $GL(2n, \mathbb{A}_F)$*, satisfying:*

- $\omega_{I_E^F(\pi)} = \omega_\pi|_{\mathbb{A}_F^*}$.
- *The image consists* PRECISELY *of the* Π *such that* $\Pi = \Pi \otimes \omega_{E/F}$.
- *If* π *is cuspidal,* $I_E^F(\pi)$ *is cuspidal if and only if* $\pi \neq \pi^\theta$.

Proof. This is due to Arthur and Clozel. See section 6 of chapter 3 in [AC]. □

For the sake of completeness, let us mention a few links between base change and automorphic induction. For any two cuspidal π and Π as above, we have:

$$I_E^F(\Pi_E) = \Pi \boxplus (\Pi \otimes \omega_{E/F}), \quad I_E^F(\pi)_E = \pi \boxplus \pi^\theta.$$

3.3 Conjugate self-dual twists

Let us now take any CM extension E/F, and consider Π_E, where Π is the theta series lifting of our original globally generic π on GSp(4). We will assume π_{v_0} is of (twisted) Steinberg type at some finite place v_0 of F. Hence Π_{E,w_0} is Steinberg at all places w_0 of E dividing v_0, and this ensures Π_E is cuspidal. In [HT], one associates Galois representations to certain *conjugate self-dual* representations. Π_E itself may not satisfy this condition, when $\omega_{\pi,E} \neq 1$, but certain twists *do*:

$$\Pi_E(\chi)^\theta \simeq \Pi_E(\chi)^\vee \Leftrightarrow \chi|_{\mathbb{A}_F^*} = \omega_\pi^{-1}\omega_{E/F}^n,$$

for $n = 0$ or $n = 1$. Such Hecke characters χ of E exist: Indeed, by Frobenius reciprocity, any Hecke character of F has infinitely many extensions to E; they are precisely the constituents of the induced representation of the compact idele class group C_E^1. By modifying this argument slightly, one can even control the ramification of the extensions if need be. Now, recall that for every place $v|\infty$,

$$\omega_{\pi_v}(a) = a^{-w},$$

for all $a \in \mathbb{R}^*$. Therefore, to retain algebraicity, take $n = 0$ above. In this case, it follows that *all* the extensions χ are automatically algebraic. That is,

$$\chi_w(z) = z^a \bar{z}^b, \quad a = a(w) \in \mathbb{Z}, \quad b = b(w) \in \mathbb{Z}, \quad a + b = w,$$

for each infinite place w of E, not to be confused with the weight! For such characters χ, the twist $\Pi_E(\chi)$ remains regular algebraic, and the weight is *zero*.

4 Galois representations

4.1 Galois representations over CM extensions

Let E be an arbitrary CM extension of the totally real field F. One of the ultimate goals of the *book* project [Har], is to attach an ℓ-adic Galois representation $\rho_{\Pi,\iota}$ to a regular algebraic conjugate self-dual cuspidal automorphic representation Π of $\mathrm{GL}(n, \mathbb{A}_E)$, and a choice of an isomorphism $\iota : \bar{\mathbb{Q}}_\ell \to \mathbb{C}$. See *expected* Theorem 2.4 in [Har] for a more precise formulation. In the case where Π has a square-integrable component at some finite place, pioneering work on this problem was done by Clozel [Cl] and Kottwitz [Kot], relating $\rho_{\Pi,\iota}|_{W_{E_w}}$ to the unramified component Π_w at most places w. Their work was later extended to all places $w \nmid \ell$ in [HT], by Harris and Taylor, in the course of proving the local Langlands conjecture. However, in [HT] the *monodromy* operator is ignored. This issue has been taken care of by Taylor and Yoshida in [TY], resulting in:

Theorem 5. *Let E be a CM extension of a totally real field F, and let Π be a cuspidal automorphic representation of $GL(n, \mathbb{A}_E)$ satisfying the conditions:*

- Π_∞ *is regular algebraic,* $H^\bullet(\mathfrak{g}, K; \Pi_\infty \otimes \mathcal{V}^*) \neq 0$.
- Π *is conjugate self-dual,* $\Pi^\vee \simeq \Pi^\theta$.
- Π_{w_0} *is (essentially) square integrable for some finite place* w_0.

Fix an isomorphism $\iota : \bar{\mathbb{Q}}_\ell \to \mathbb{C}$. Then there is a continuous representation

$$\rho_{\Pi,\iota} : Gal(\bar{F}/E) \to GL(n, \bar{\mathbb{Q}}_\ell)$$

such that for every finite place w of E, not dividing ℓ, we have the following:

$$\iota WD(\rho_{\Pi,\iota}|_{W_{E_w}})^{F-ss} \simeq rec_n(\Pi_w \otimes |\det|^{\frac{1-n}{2}}).$$

Proof. This is Theorem 1.2 in [TY], which is a refinement of Theorem VII.1.9 in [HT]. Indeed, the former result identifies the monodromy operator: By Corollary VII.1.11 in [HT] it is known that Π_w is *tempered* for all finite places w. Therefore, by parts (3) and (4) of Lemma 1.4 in [TY], it suffices to show that $\iota\mathrm{WD}(\rho_{\Pi,\iota}|_{W_{E_w}})$ is *pure*. That is, up to a shift, the weight filtration coincides with the monodromy filtration. This is proved in [TY] by a careful study of the Rapoport-Zink weight spectral sequence, the main new ingredient being the vanishing outside the middle-degree in Proposition 4.4 in [TY]. □

A word about the notation used in the previous Theorem: First, $\mathcal{V}$ denotes an irreducible algebraic representation over $\mathbb{C}$ of the group $R_{E/\mathbb{Q}}\mathrm{GL}(n)$, which we will denote by $\mathcal{G}$. Then $\mathfrak{g}$ denotes the Lie algebra of $\mathcal{G}(\mathbb{R})$, and K is a maximal compact subgroup times $Z_{\mathcal{G}}(\mathbb{R})$. The symbol $WD(\rho)$ stands for the Weil-Deligne representation corresponding to an ℓ-adic representation ρ of W_{E_w}, where $w \nmid \ell$. This pair (r, N) is obtained by fixing a lift Frob_w of the geometric Frobenius, and a continuous surjective homomorphism $t_\ell : I_{E_w} \to \mathbb{Z}_\ell$, and then writing

$$\rho(\mathrm{Frob}_w^m \sigma) = r(\mathrm{Frob}_w^m \sigma)\exp(t_\ell(\sigma)N)$$

for $\sigma \in I_{E_w}$ and integers m. Then r is a representation of W_{E_w} having an *open* kernel, and N is a nilpotent operator satisfying the formula mentioned above:

$$N \circ r(\mathrm{Frob}_w) = q_w \cdot r(\mathrm{Frob}_w) \circ N.$$

Here q_w is the order of the residue field of E_w. The isomorphism class of (r, N) is independent of the choices made. Finally, the superscript $F - ss$ signifies Frobenius *semisimplification*. That is, leave N unchanged, but semisimplify r. The representations $\rho_{\Pi,\iota}$ above satisfy a number of additional nice properties:

- Π is square integrable at some finite $w_0 \nmid \ell \Longrightarrow \rho_{\Pi,\iota}$ is irreducible.
- Let $w \nmid \ell$ be a finite place of E, and let α be an eigenvalue of $\rho_{\Pi,\iota}(\sigma)$ for some $\sigma \in W_{E_w}$. Then α belongs to $\bar{\mathbb{Q}}$, and for every embedding $\bar{\mathbb{Q}} \hookrightarrow \mathbb{C}$,
$$|\alpha| \in q_w^{\frac{\mathbb{Z}}{2}}.$$
- Let $w \nmid \ell$ be a finite place, with Π_w *unramified*, and let α be an eigenvalue of $\rho_{\Pi,\iota}(\mathrm{Frob}_w)$. Then α belongs to $\bar{\mathbb{Q}}$, and for every embedding $\bar{\mathbb{Q}} \hookrightarrow \mathbb{C}$,
$$|\alpha| = q_w^{\frac{n-1}{2}}.$$
- The representation $\rho_{\Pi,\iota}$ is potentially semistable at any finite place $w|\ell$. Moreover, $\rho_{\Pi,\iota}$ is crystalline at a finite place $w|\ell$ when Π_w is unramified.

The first property is clear since $\mathrm{rec}_n(\Pi_{w_0} \otimes |\det|^{\frac{1-n}{2}})$ is indecomposable. This was observed in Corollary 1.3 in [TY]. It is expected to continue to hold if $w_0|\ell$ (and even without the square-integrability condition, admitting the book project). The second and the third property are parts 1 and 2 of Theorem VII.1.9 in [HT]. The former is a special case of Lemma I.5.7 in [HT], which apparently follows from the Rapoport-Zink weight spectral sequence in conjunction with de Jong's theory of alterations. The latter follows from Deligne's work on the Weil conjectures. The last property comes down to the comparison theorems of p-adic Hodge theory. To clarify these comments, we will briefly sketch how $\rho_{\Pi,\iota}$ is realized geometrically in [HT]: One starts off with an n^2-dimensional central division algebra B over E, equipped with a positive involution $*$ such that $*|_E = \theta$. It is assumed to satisfy a list of properties, which are irrelevant for our informal discussion. For a fixed $\beta \in B$ such that $\beta\beta^* = 1$, look at the unitary similitude group G defined as follows: For a commutative $\mathbb{Q}$-algebra R,

$$G(R) = \{x \in (B^{\mathrm{op}} \otimes_{\mathbb{Q}} R)^* \colon\ x^*\beta x = c(x)\beta, \text{ with } c(x) \in R^*\}.$$

The element β is chosen such that, at infinity, the derived group takes the form

$$G^{\mathrm{der}}(\mathbb{R}) = U(n-1,1) \times U(n)^{[F:\mathbb{Q}]-1}.$$

The group G has an associated Shimura variety of PEL type. That is, for each sufficiently small compact open subgroup K inside the finite adeles $G(\mathbb{A}_f)$, there is a smooth proper variety X_K over E classifying isogeny classes of polarized abelian schemes A of dimension $[F:\mathbb{Q}]n^2$, endowed with a certain homomorphism from B into $\mathrm{End}(A)_{\mathbb{Q}}$ and a so-called level-structure relative to K. On X_K one defines a $\bar{\mathbb{Q}}_\ell$-sheaf $\mathcal{L}_\xi$ by fixing an algebraic representation ξ of G defined over $\bar{\mathbb{Q}}_\ell$. Then, consider the following direct limit over subgroups K, endowed with natural commuting actions of $G(\mathbb{A}_f)$ and of the Galois group of E:

$$H^m(X,\mathcal{L}_\xi) \stackrel{\mathrm{df}}{=} \varinjlim_K H^m_{\mathrm{et}}(X_K \times_E \bar{F}, \mathcal{L}_\xi) = \bigoplus_{\pi_f} \pi_f \otimes R^m_\xi(\pi_f).$$

Here π_f runs over the irreducible admissible representations of $G(\mathbb{A}_f)$, and $R^m_\xi(\pi_f)$ is a finite-dimensional continuous Galois representation of E. To construct $\rho_{\Pi,\iota}$, we first descend Π to an automorphic representation $\tilde{\Pi}$ of $B^{\mathrm{op},*}$ via the Jacquet-Langlands correspondence. Using results of Clozel and Labesse, one shows that $\psi \times \tilde{\Pi}$ is a base change from G, for some algebraic Hecke character ψ of E. In this way, we end up with an automorphic representation π of G, and

$$R^{n-1}_\xi(\pi_f^\vee)^{\mathrm{ss}} \simeq \rho^a_{\Pi,\iota} \otimes \rho_{\psi,\iota}$$

for some positive integer a. For details see p. 228 in [HT], and p. 12 in [TY].

4.2 Hodge-Tate weights

We will now describe the Hodge-Tate weights, which are certain numerical invariants of the restriction of $\rho_{\Pi,\iota}$ to the Galois group of E_w for each place $w|\ell$. We briefly recall their definition: Let $\mathcal{K}$ be a finite extension of $\mathbb{Q}_\ell$. Following Fontaine, we introduce the field of ℓ-adic periods B_{dR}. This is a $\mathcal{K}$-algebra, it comes equipped with a discrete valuation v_{dR}, and has residue field $\mathbb{C}_\ell$. The topology on B_{dR} is coarser than the one coming form the valuation. The Galois group of $\mathcal{K}$ acts continuously on B_{dR}. If $t \in B_{dR}$ is a uniformizer, then we have

$$g \cdot t = \chi_{\mathrm{cyc}}(g)t,$$

where χ_{cyc} is the ℓ-adic cyclotomic character. The valuation defines a filtration:

$$\mathrm{Fil}^j(B_{dR}) \stackrel{\mathrm{df}}{=} t^j B^+_{dR}, \quad \mathrm{gr}^j(B_{DR}) \stackrel{\mathrm{df}}{=} \mathrm{Fil}^j(B_{dR})/\mathrm{Fil}^{j+1}(B_{dR}) \simeq \mathbb{C}_\ell(j).$$

If V is a finite-dimensional continuous $\bar{\mathbb{Q}}_\ell$-representation of $\mathrm{Gal}(\bar{\mathbb{Q}}_\ell/\mathcal{K})$, we let

$$D_{dR}(V) \stackrel{\mathrm{df}}{=} (V \otimes_{\mathbb{Q}_\ell} B_{dR})^{\mathrm{Gal}(\bar{\mathbb{Q}}_\ell/\mathcal{K})}.$$

This is a module over $\bar{\mathbb{Q}}_\ell \otimes_{\mathbb{Q}_\ell} \mathcal{K}$, inheriting a filtration from B_{dR}. We say that V is *de Rham* if this module is free of rank $\dim_{\bar{\mathbb{Q}}_\ell}(V)$. In this case, for each embedding $\tau : \mathcal{K} \to \bar{\mathbb{Q}}_\ell$ we introduce a multiset of integers $\mathrm{HT}_\tau(V)$. It contains $\dim_{\bar{\mathbb{Q}}_\ell}(V)$ elements, and j occurs with multiplicity equal to the dimension of

$$\mathrm{gr}^j(V \otimes_{\tau,\mathcal{K}} B_{dR})^{\mathrm{Gal}(\bar{\mathbb{Q}}_\ell/\mathcal{K})} = \mathrm{gr}^j D_{dR}(V) \otimes_{\bar{\mathbb{Q}}_\ell \otimes_{\mathbb{Q}_\ell} \mathcal{K}, 1\otimes\tau} \bar{\mathbb{Q}}_\ell.$$

over $\bar{\mathbb{Q}}_\ell$. If this is nonzero, j is called a *Hodge-Tate* weight for V relative to the embedding τ. Now we specialize the discussion, and take V to be the restriction of $\rho_{\Pi,\iota}$ as above. We will quote a result from [HT], as stated in [Har], relating the Hodge-Tate weights to the highest weights of the algebraic representation $\mathcal{V}^*$. Recall, this is the irreducible algebraic representation of $\mathcal{G}(\mathbb{C})$ such that the tensor product $\Pi_\infty \otimes \mathcal{V}^*$ has cohomology. By the definition of the $\mathbb{Q}$-group $\mathcal{G}$,

$$\mathcal{G}(\mathbb{R}) = \prod_{\sigma\in\Sigma} \mathrm{GL}_n(E \otimes_{F,\sigma} \mathbb{R}), \quad \mathcal{G}(\mathbb{C}) = \prod_{\sigma\in\Sigma} \mathrm{GL}_n(E \otimes_{F,\sigma} \mathbb{C}),$$

where Σ is the set of embeddings $\sigma : F \to \mathbb{R}$. For each such σ, following [Har], we let $\{\tilde{\sigma}, \tilde{\sigma}^c\}$ denote the two complex embeddings of E extending it. We write

$$\mathcal{V}^* = \otimes_{\sigma\in\Sigma} \mathcal{V}^*_\sigma, \quad \mathcal{V}^*_\sigma = \mathcal{V}^*_{\tilde{\sigma}} \otimes \mathcal{V}^*_{\tilde{\sigma}^c}.$$

Here $\mathcal{V}^*_{\tilde{\sigma}}$ is naturally identified with an irreducible algebraic representation of the group $\mathrm{GL}_n(\mathbb{C})$, and we consider its highest weight relative to the *lower* triangular Borel. This is the character of the diagonal torus corresponding to

$$\mu(\tilde{\sigma}) = (\mu_1(\tilde{\sigma}) \leq \mu_2(\tilde{\sigma}) \leq \cdots \leq \mu_n(\tilde{\sigma})).$$

Similarly, we get a dominant n-tuple of integers $\mu(\tilde{\sigma}^c)$ for $\mathcal{V}^*_{\tilde{\sigma}^c}$. It is given by:

$$\mu_i(\tilde{\sigma}^c) = -\mu_{n-i+1}(\tilde{\sigma}),$$

by the polarization condition. The multisets HT_τ for $\rho_{\Pi,\iota}$ are determined by:

Theorem 6. *Fix an embedding $s : E \to \bar{\mathbb{Q}}_\ell$, and let w denote the associated finite place of E above ℓ. Then the Hodge-Tate weights of $\rho_{\Pi,\iota}$ restricted to the Galois group $Gal(\bar{\mathbb{Q}}_\ell/E_w)$ at w, where $E_w = s(E)^-$, are all of the form*

$$j = i - \mu_{n-i}(\iota(s)^c), \quad i = 0, \ldots, n-1.$$

In particular, the Hodge-Tate weights all occur with multiplicity one.

Proof. This is part 4 of Theorem VII.1.9 on p. 227 in [HT], but with the normalization used in [Har] in (2.6) on p. 5: The shift from $\iota(s)$ to $\iota(s)^c$ reflects the fact that we work with the *dual* of the Π in [HT]. Note that the inequalities on p. 3 in [Har] should be reversed. $\square$

4.3 Patching

The next key step is to *descend* the family $\rho_{\Pi_E(\chi),\iota} \otimes \chi^{-1}$ to the base field F. This is done by a patching argument, used in various guises by other authors. For example, see Proposition 4.3.1 in [BRo], or section 4.3 in [BRa]. Here we will use a variant of Proposition 1.1 in [Har], which in turn is based on the discussion on p. 230-231 in [HT]. The proof in [Har] is somewhat brief, and somewhat imprecise at the end, so we decided to include a more detailed proof below. Hopefully, this might serve as a convenient reference. In this section, we use Γ_F as shorthand notation for the absolute Galois group $\mathrm{Gal}(\bar{F}/F)$. The setup is the following: We let $\mathcal{I}$ be a set of cyclic Galois extensions E, of a fixed number field F, of *prime* degree q_E. For every $E \in \mathcal{I}$ we assume we are given an n-dimensional continuous semisimple ℓ-adic Galois representation over E,

$$\rho_E : \Gamma_E \to \mathrm{GL}_n(\bar{\mathbb{Q}}_\ell).$$

Here ℓ is a fixed prime. The family of representations $\{\rho_E\}$ is assumed to satisfy:

(a) Galois invariance: $\rho_E^\sigma \simeq \rho_E, \quad \forall \sigma \in \mathrm{Gal}(E/F)$,

(b) Compatibility: $\rho_E|_{\Gamma_{EE'}} \simeq \rho_{E'}|_{\Gamma_{EE'}}$,

for all E and E' in $\mathcal{I}$. These conditions are certainly necessary for the ρ_E to be of the form $\rho|_{\Gamma_E}$ for a representation ρ of Γ_F. What we will show, is that in fact (a) and (b) are also sufficient conditions if $\mathcal{I}$ is large enough. That is,

Definition 1. *Following [Har], for a finite set S of places of F, we say that $\mathcal{I}$ is S-general if and only if the following holds: For any finite place $v \notin S$, and any finite extension M of F, there is an $E \in \mathcal{I}$ linearly disjoint from M such that v splits completely in E. In this case, there will be infinitely many such E.*

Recall that since E is Galois over F, it is linearly disjoint from M precisely when $E \cap M = F$. Moreover, it is of prime degree, so this just means E is not contained in M. Hence, $\mathcal{I}$ being S-general is equivalent to: For $v \notin S$, there are infinitely many $E \in \mathcal{I}$ in which v splits. A slightly stronger condition is:

Definition 2. *We say that $\mathcal{I}$ is strongly S-general if and only if the following holds: For any finite set Σ of places of F, disjoint from S, there is an $E \in \mathcal{I}$ in which every $v \in \Sigma$ splits completely.*

To see that this is indeed *stronger*, we follow Remark 1.3 in [Har]: Fix a finite place $v \notin S$, and a finite extension M of F. Clearly we may assume $M \neq F$ is Galois. Let $\{M_i\}$ be the subfields of M, Galois over F, with a simple Galois group. For each i we then choose a place v_i of F, not in S, which does *not* split completely in M_i. We take Σ to be $\{v, v_i\}$ in the above definition, and get an $E \in \mathcal{I}$ in which v and every v_i splits. If E was contained in M, it would be one of the M_i, but this contradicts the choice of v_i. Thus, E and M are disjoint.

Example. Let $\Sigma = \{p_i\}$ be a finite set of primes. As is well-known, for odd p_i,

$$p_i \text{ splits in } \mathbb{Q}(\sqrt{d}) \Longleftrightarrow p_i \nmid d \text{ and } \left(\frac{d}{p_i}\right) = 1.$$

Here d is any square-free integer. Moreover, 2 splits when $d \equiv 1 \bmod 8$. The set of *all* integers d satisfying the congruences $d \equiv 1 \bmod p_i$, for all i, form an arithmetic progression. By Dirichlet's Theorem, it contains infinitely many primes. Therefore, the following family of imaginary quadratic extensions

$$\mathcal{I} = \{\mathbb{Q}(\sqrt{-p})\text{: almost all primes } p\}$$

is strongly $\varnothing$-general. This gives rise to a similar family of CM extensions of any given totally real field F, by taking the set of all the composite fields $F\mathcal{I}$.

The main result of this section, is a strengthening of Proposition 1.1 in [Har]:

Lemma 1. *Let $\mathcal{I}$ be an S-general set of extensions E over F, of prime degree q_E, and let ρ_E be a family of semisimple Galois representations satisfying the conditions (a) and (b) above. Then there is a continuous semisimple*

$$\rho : \Gamma_F \to GL_n(\bar{\mathbb{Q}}_\ell), \quad \rho|_{\Gamma_E} \simeq \rho_E,$$

for all $E \in \mathcal{I}$. *This determines the representation ρ uniquely up to isomorphism.*

Proof. The proof below is strongly influenced by the proofs of Proposition 1.1 in [Har], and of Theorem VII.1.9 in [HT]. We simply include more details and clarifications. The proof is quite long and technical, so we divide it into several steps. Before we construct ρ, we start off with noting that it is necessarily *unique*: Indeed, for any place $v \notin S$, we find an $E \in \mathcal{I}$ in which v splits. In particular, $E_w = F_v$ for all places w of E dividing v. Thus, all the restrictions $\rho|_{\Gamma_{F_v}}$ are uniquely determined. We conclude that ρ is unique, by the Cebotarev Density Theorem. For the construction of ρ, we first establish some *notation* used throughout the proof: We fix an arbitrary *base* point $E_0 \in \mathcal{I}$, and abbreviate

$$\rho_0 \overset{\text{df}}{=} \rho_{E_0}, \quad \Gamma_0 \overset{\text{df}}{=} \Gamma_{E_0}, \quad G_0 \overset{\text{df}}{=} \mathrm{Gal}(E_0/F), \quad q_0 \overset{\text{df}}{=} q_{E_0}.$$

We let H denote the Zariski closure of $\rho_0(\Gamma_0)$ inside $\mathrm{GL}_n(\bar{\mathbb{Q}}_\ell)$, and consider its identity component H°. Define M to be the finite Galois extension of E_0 with

$$\Gamma_M = \rho_0^{-1}(H^\circ), \quad \mathrm{Gal}(M/E_0) = \pi_0(H).$$

Let T be the set of isomorphism classes of irreducible constituents of ρ_0, ignoring multiplicities. By property (a), the group G_0 acts on T from the right. We note that τ and τ^σ occur in ρ_0 with the same multiplicity. We want to describe the G_0-orbits on T. First, we have the set P of fixed points $\tau = \tau^\sigma$ for all σ.

The set of non-trivial orbits is denoted by C. Note that any $c \in C$ has prime cardinality q_0. For each such c, we pick a representative $\tau_c \in T$, and let C_0 be the set of all these representatives $\{\tau_c\}$. Each $\tau \in C_0$ obviously has a trivial stabilizer in G_0.

Step 1: *The extensions of ρ_0 to Γ_F.*

Firstly, a standard argument shows that each $\tau \in P$ has an extension $\tilde{\tau}$ to Γ_F. This uses the divisibility of $\bar{\mathbb{Q}}_\ell^*$, in order to find a suitable intertwining operator $\tau \simeq \tau^\sigma$. All the other extensions are then obtained from $\tilde{\tau}$ as unique twists:

$$\tilde{\tau} \otimes \eta, \quad \eta \in \hat{G}_0.$$

Here $\hat{G}_0$ is the group of characters of G_0. Secondly, for a $\tau \in c$, we introduce

$$\tilde{\tau} \stackrel{\mathrm{df}}{=} \mathrm{Ind}_{\Gamma_0}^{\Gamma_F}(\tau).$$

Since τ is *not* Galois-invariant, this $\tilde{\tau}$ is irreducible. It depends only on the orbit c containing τ, and it is invariant under twisting by $\hat{G}_0$. It has restriction

$$\tilde{\tau}|_{\Gamma_0} \simeq \bigoplus\nolimits_{\sigma \in G_0} \tau^\sigma.$$

If we let m_τ denote the multiplicity with which $\tau \in T$ occurs in ρ_0, we get that

$$\{\bigoplus_{\tau \in C_0} m_\tau \cdot \tilde{\tau}\} \oplus \{\bigoplus_{\tau \in P} \bigoplus\nolimits_{\eta \in \hat{G}_0} m_{\tilde{\tau},\eta} \cdot (\tilde{\tau} \otimes \eta)\}$$

is an extension of ρ_0 to Γ_F for all choices of non-negative $m_{\tilde{\tau},\eta} \in \mathbb{Z}$ such that

$$\sum\nolimits_{\eta \in \hat{G}_0} m_{\tilde{\tau},\eta} = m_\tau$$

for every fixed $\tau \in P$.

Step 2: *$\rho_0(\Gamma_{NE_0})$ is dense in H, when N is linearly disjoint from M over F.*

To see this, let us momentarily denote the Zariski closure of $\rho_0(\Gamma_{NE_0})$ by H_N. N is a finite extension, so H_N has finite index in H. Consequently, we deduce that $H_N^\circ = H^\circ$. Now, NE_0 and M are linearly disjoint over E_0, and therefore

$$\Gamma_0 = \Gamma_{NE_0} \cdot \Gamma_M \Longrightarrow \rho_0(\Gamma_0) \subset \rho_0(\Gamma_{NE_0}) \cdot H^\circ \subset H_N.$$

Taking the closure, we obtain that $H_N = H$.

Step 3: *If N is a finite extension of F, linearly disjoint from M over F. Then:*

(1) $\tau|_{\Gamma_{NE_0}}$ is irreducible, for all $\tau \in T$.

(2) $\tilde{\tau}|_{\Gamma_N}$ is irreducible, for all $\tau \in P$.

(3) $\tau|_{\Gamma_{NE_0}} \simeq \tau'|_{\Gamma_{NE_0}} \Rightarrow \tau \simeq \tau'$, for all $\tau, \tau' \in T$.

(4) $\tilde{\tau}|_{\Gamma_N} \simeq (\tilde{\tau}' \otimes \eta)|_{\Gamma_N} \Rightarrow \tau \simeq \tau'$ *and* $\eta = 1$*, for all* $\tau, \tau' \in P$ *and* $\eta \in \hat{G}_0$*.*

Parts (1) and (3) follow immediately from Step 2, and obviously (1) implies (2). Also, part (3) immediately implies that $\tau \simeq \tau'$ in (4). Suppose $\eta \in \hat{G}_0$ satisfies:

$$\tilde{\tau}|_{\Gamma_N} \simeq \tilde{\tau}|_{\Gamma_N} \otimes \eta|_{\Gamma_N}$$

for some $\tau \in P$. In other words, $\eta|_{\Gamma_N}$ occurs in $\mathrm{End}_{\Gamma_{NE_0}}(\tilde{\tau}|_{\Gamma_N})$, which is trivial by part (1). So, η is trivial on Γ_N and on Γ_0. Hence, $\eta = 1$ by disjointness.

Step 4: *$\tilde{\tau}|_{\Gamma_N}$ is irreducible for all $\tau \in C_0$. That is, part (2) holds for all $\tau \in T$.*

Since N and E_0 are linearly disjoint over F, we see that $\Gamma_F = \Gamma_E \cdot \Gamma_0$. Hence,

$$\tilde{\tau}|_{\Gamma_N} = \mathrm{Ind}_{\Gamma_0}^{\Gamma_F}(\tau)|_{\Gamma_N} \simeq \mathrm{Ind}_{\Gamma_{NE_0}}^{\Gamma_N}(\tau|_{\Gamma_{NE_0}}),$$

by Mackey theory. Now, $\tau|_{\Gamma_{NE_0}}$ is irreducible and *not* Galois-invariant.

Step 5: *Suppose $E \in \mathcal{I}$ is linearly disjoint from M over F. Then, for a unique choice of non-negative integers $m_{\tilde{\tau},\eta,E}$ with η-sum m_τ, we have the formula:*

$$\rho_E \simeq \{\bigoplus_{\tau \in C_0} m_\tau \cdot \tilde{\tau}|_{\Gamma_E}\} \oplus \{\bigoplus_{\tau \in P} \bigoplus\nolimits_{\eta \in \hat{G}_0} m_{\tilde{\tau},\eta,E} \cdot (\tilde{\tau} \otimes \eta)|_{\Gamma_E}\}.$$

In particular, ρ_0 and ρ_E have a <u>common</u> extension to Γ_F.

The uniqueness of the $m_{\tilde{\tau},\eta,E}$ follows directly from part (4) in Step 3. Recall,

$$\rho_E|_{\Gamma_{EE_0}} \simeq \rho_0|_{\Gamma_{EE_0}} \simeq \{\bigoplus_{\tau \in C_0} m_\tau \cdot \bigoplus\nolimits_{\sigma \in G_0} \tau|^{\sigma}_{\Gamma_{EE_0}}\} \oplus \{\bigoplus_{\tau \in P} m_\tau \cdot \tau|_{\Gamma_{EE_0}}\},$$

by the compatibility condition (b). Here all the $\tau|^{\sigma}_{\Gamma_{EE_0}}$ are distinct by (3). First, let us pick an arbitrary $\tau \in P$. As representations of G_0, viewed as the Galois group of EE_0 over E by disjointness, we have

$$\mathrm{Hom}_{\Gamma_{EE_0}}(\tilde{\tau}|_{\Gamma_E}, \rho_E) \simeq \bigoplus\nolimits_{\eta \in \hat{G}_0} \dim_{\bar{\mathbb{Q}}_\ell} \mathrm{Hom}_{\Gamma_E}((\tilde{\tau} \otimes \eta)|_{\Gamma_E}, \rho_E) \cdot \eta.$$

The $\bar{\mathbb{Q}}_\ell$-dimension of the left-hand side clearly equals m_τ, and the right-hand side defines the partition $m_{\tilde{\tau},\eta,E}$ of m_τ. Next, let us pick an arbitrary $\tau \in C_0$. By the same argument, using that $\tilde{\tau}$ is invariant under twisting by $\hat{G}_0$, we get:

$$\mathrm{Hom}_{\Gamma_{EE_0}}(\tilde{\tau}|_{\Gamma_E}, \rho_E) \simeq \dim_{\bar{\mathbb{Q}}_\ell} \mathrm{Hom}_{\Gamma_E}(\tilde{\tau}|_{\Gamma_E}, \rho_E) \cdot \bigoplus\nolimits_{\eta \in \hat{G}_0} \eta.$$

Now the left-hand side obviously has dimension $m_\tau q_0$. We deduce that $\tilde{\tau}|_{\Gamma_E}$ occurs in ρ_E with multiplicity m_τ. Counting dimensions, we obtain the desired decomposition of ρ_E. Note that we have not used the Galois invariance of ρ_E. In fact, it is a *consequence* of the above argument, assuming $E \cap M = F$.

Step 6: *Fix an $E_1 \in \mathcal{I}$ disjoint from M over F. Introduce the representation*

$$\rho \stackrel{\text{df}}{=} \{\bigoplus_{\tau \in C_0} m_\tau \cdot \tilde{\tau}\} \oplus \{\bigoplus_{\tau \in P} \bigoplus\nolimits_{\eta \in \hat{G}_0} m_{\tilde{\tau},\eta,E_1} \cdot (\tilde{\tau} \otimes \eta)\}.$$

Then $\rho|_{\Gamma_E} \simeq \rho_E$ for all extensions $E \in \mathcal{I}$ linearly disjoint from ME_1 over F.

By definition, and Step 5, we have that $\rho|_{\Gamma_{E_1}} \simeq \rho_{E_1}$. Take $E \in \mathcal{I}$ to be any extension, disjoint from ME_1 over F. We compare the decomposition of $\rho|_{\Gamma_E}$,

$$\rho|_{\Gamma_E} = \{\bigoplus_{\tau \in C_0} m_\tau \cdot \tilde{\tau}|_{\Gamma_E}\} \oplus \{\bigoplus_{\tau \in P} \bigoplus\nolimits_{\eta \in \hat{G}_0} m_{\tilde{\tau},\eta,E_1} \cdot (\tilde{\tau} \otimes \eta)|_{\Gamma_E}\},$$

to the decomposition of ρ_E in Step 5. We need to show the multiplicities match:

$$m_{\tilde{\tau},\eta,E} = m_{\tilde{\tau},\eta,E_1}, \quad \forall \tau \in P, \quad \forall \eta \in \hat{G}_0.$$

By property (b), for the pair $\{E, E_1\}$, we know that $\rho|_{\Gamma_E}$ and ρ_E become isomorphic after restriction to Γ_{EE_1}. Once we prove EE_1 is linearly disjoint from M over F, we are done by (2) and (4). The disjointness folllows immediately:

$$EE_1 \otimes_F M \simeq E \otimes_F E_1 \otimes_F M \simeq E \otimes_F ME_1 \simeq EE_1M.$$

Step 7: *$\rho|_{\Gamma_E} \simeq \rho_E$ for* all *$E \in \mathcal{I}$.*

By Step 6, we may assume $E \in \mathcal{I}$ is *contained* in ME_1. Now take an auxiliary extension $\mathcal{E} \in \mathcal{I}$ linearly disjoint from ME_1 over F. Consequently, using (b),

$$\rho|_{\Gamma_{\mathcal{E}}} \simeq \rho_{\mathcal{E}} \Rightarrow \rho|_{\Gamma_{E\mathcal{E}}} \simeq \rho_{\mathcal{E}}|_{\Gamma_{E\mathcal{E}}} \simeq \rho_E|_{\Gamma_{E\mathcal{E}}}.$$

Thus, $\rho|_{\Gamma_E}$ agrees with ρ_E when restricted to $\Gamma_{E\mathcal{E}}$. It suffices to show that the union of these subgroups $\Gamma_{E\mathcal{E}}$, as $\mathcal{E}$ varies, is dense in Γ_E. Again, we invoke the Cebotarev Density Theorem. Indeed, let w be a place of E, lying above $v \notin S$. It is then enough to find an $\mathcal{E} \in \mathcal{I}$, as above, such that w splits completely in $E\mathcal{E}$. Then Γ_{E_w} is contained in $\Gamma_{E\mathcal{E}}$. We *know*, by the S-generality of $\mathcal{I}$, that we can find an $\mathcal{E} \in \mathcal{I}$, not contained in ME_1, in which v splits completely. This $\mathcal{E}$ works: This follows from elementary splitting theory, as E and $\mathcal{E}$ are disjoint.

This finishes the proof of the patching lemma. □

Remark. From the proof above, we infer the following concrete description of the patch-up representation ρ. First fix *any* $E_0 \in \mathcal{I}$, and let P be the set of Galois-invariant constituents τ of ρ_{E_0}. For each such τ, we fix an extension $\tilde{\tau}$ to F once and for all. Furthermore, let C_0 be a set of representatives for the non-trivial Galois orbits of constituents of ρ_{E_0}. Then ρ is of the following form

$$\rho \simeq \{\bigoplus_{\tau \in C_0} m_\tau \cdot \mathrm{Ind}_{\Gamma_0}^{\Gamma_F}(\tau)\} \oplus \{\bigoplus_{\tau \in P} \bigoplus\nolimits_{\eta \in \mathrm{Gal}(E_0/F)^\wedge} m_{\tilde{\tau},\eta} \cdot (\tilde{\tau} \otimes \eta)\}.$$

Here the $m_{\tilde{\tau},\eta}$ are *some* non-negative integers with η-sum m_τ, the multiplicity of τ in ρ_{E_0}. This fairly explicit description may be useful in deriving properties of ρ from those of ρ_{E_0}.

For future reference, we finish this section with a few remarks on the generalization of the patching lemma to *solvable* extensions. Thus, $\mathcal{I}$ now denotes a collection of solvable Galois extensions E over F, and we assume we are given Galois representations ρ_E, as above, satisfying (a) and (b). For any L over F,

$$\mathcal{I}_L \stackrel{\text{df}}{=} \{E \in \mathcal{I} : L \subset E\}.$$

Loosely speaking, we say that $\mathcal{I}$ is S-general if it is S-general in prime layers:

Definition 3. *Following [Har], for a finite set S of places of F, we say that $\mathcal{I}$ is S-general if and only if the following holds: For every L such that $\mathcal{I}_L \neq \varnothing$,*

$$\{\textit{prime degree extensions } K/L, \textit{ with } \mathcal{I}_K \neq \varnothing\}$$

is $S(L)$-general in the previous sense. $S(L)$ denotes the places of L above S.

From now on, we will make the additional hypothesis that all the extensions $E \in \mathcal{I}$ have uniformly *bounded heights*. That is, there is an integer $H_{\mathcal{I}}$ such that every index $[E : F]$ has at most $H_{\mathcal{I}}$ prime divisors (not necessarily distinct).

Lemma 2. *Assume the collection $\mathcal{I}$ has uniformly bounded heights. Then $\mathcal{I}$ is S-general if and only if the following condition holds for every L with $\mathcal{I}_L \neq \varnothing$: Given a finite place $w \notin S(L)$ and a finite extension M over L, there is an extension $E \in \mathcal{I}_L$ linearly disjoint from M over L, in which w splits completely.*

Proof. The *if* part follows immediately by unraveling the definitions. The *only if* part is proved by induction on the maximal height of the collection $\mathcal{I}_L$ over L, the height *one* case being the definition. Suppose $\mathcal{I}_L$ has maximal height H, and assume the lemma holds for smaller heights. Let w and M be as above. By S-generality, there is a prime degree extension K over L with $\mathcal{I}_K \neq \varnothing$, disjoint from M over L, in which w splits. Fix a place $\tilde{w}$ of K above w. Now, $\mathcal{I}_K$ clearly has maximal height *less* than H. By the induction hypothesis there is an $E \in \mathcal{I}_K$, disjoint from MK over K, in which $\tilde{w}$ splits. This E works. □

Under the above assumptions on $\mathcal{I}$, a given place $w \notin S(L)$ splits completely in infinitely many $E \in \mathcal{I}_L$, unless L belongs to $\mathcal{I}$. One has a stronger notion:

Definition 4. *We say that $\mathcal{I}$ is strongly S-general if and only if the following holds: For any L such that $\mathcal{I}_L \neq \varnothing$, and any finite set Σ of places of L disjoint from $S(L)$, there is an $E \in \mathcal{I}_L$ in which every $v \in \Sigma$ splits completely.*

As in the prime degree case, treated above, one shows that this is indeed a stronger condition. Our next goal is to prove the following generalization of the patching lemma to certain collections of solvable extensions:

Theorem 7. *Let $\mathcal{I}$ be an S-general collection of solvable Galois extensions E over F, with uniformly bounded heights, and let ρ_E be a family of n-dimensional continuous semisimple ℓ-adic Galois representations satisfying the conditions (a) and (b) above. Then there is a continuous semisimple representation*

$$\rho : \Gamma_F \to GL_n(\bar{\mathbb{Q}}_\ell), \quad \rho|_{\Gamma_E} \simeq \rho_E,$$

for ALL $E \in \mathcal{I}$. *This determines the representation ρ uniquely up to isomorphism.*

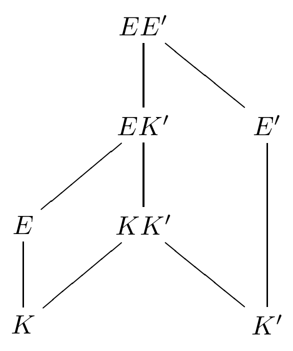
Proof. Uniqueness is proved by paraphrasing the argument in the prime degree situation. The existence of ρ is proved by induction on the maximal height of $\mathcal{I}$ over F, the height one case being the previous patching lemma. Suppose $\mathcal{I}$ has maximal height H, and assume the Theorem holds for smaller heights. Take an arbitrary prime degree extension K over F, with $\mathcal{I}_K \neq \varnothing$. Clearly $\mathcal{I}_K$ is an $S(K)$-general set of solvable Galois extensions of K, of maximal height strictly smaller than H. Moreover, the subfamily $\{\rho_E\}_{E \in \mathcal{I}_K}$ obviously satisfies (a) and (b). By induction, we find a continuous semisimple ℓ-adic representation

$$\rho_K : \Gamma_K \to \mathrm{GL}_n(\bar{\mathbb{Q}}_\ell), \quad \rho_K|_{\Gamma_E} \simeq \rho_E,$$

for all $E \in \mathcal{I}_K$. We then wish to apply the prime degree patching lemma to the family $\{\rho_K\}$, as K varies over extensions as above. By definition, such K do form an S-general collection over F. It remains to show that $\{\rho_K\}$ satisfies (a) and (b). To check property (a), take any $\sigma \in \Gamma_F$, and note that ρ_K^σ agrees with ρ_K after restriction to Γ_E for an arbitrary extension $E \in \mathcal{I}_K$. The union of these Γ_E is dense in Γ_K by the Cebotarev Density Theorem: Every place w of K, outside $S(K)$, splits in some $E \in \mathcal{I}_K$, so the union contains Γ_{K_w}. To check property (b), fix prime degree extensions K and K' as above. Note that

$$(\rho_K|_{\Gamma_{KK'}})|_{\Gamma_{EE'}} \simeq (\rho_{K'}|_{\Gamma_{KK'}})|_{\Gamma_{EE'}}, \quad \forall E \in \mathcal{I}_K, \quad \forall E' \in \mathcal{I}_{K'}.$$

We finish the proof by showing that the union of these $\Gamma_{EE'}$ is dense in $\Gamma_{KK'}$. Let w be an arbitrary place of KK' such that $w|_F$ does not lie in S. Choose an extension $E \in \mathcal{I}_K$ linearly disjoint from KK' over K, in which $w|_K$ splits. Then pick an extension $E' \in \mathcal{I}_{K'}$ linearly disjoint from EK' over K', in which $w|_{K'}$ splits. By elementary splitting theory, w splits in EK', and any place of EK' above w splits in EE'. Consequently, w splits in EE', see the diagram:



The union then contains the Galois group of $(KK')_w$. Done by Cebotarev. $\square$

The previous result should be compared to Corollary 1.2 in [Har].

4.4 Galois representations associated to π

Let π be the globally generic cusp form on GSp(4) introduced earlier, Π its lift to GL(4), and let Π_E be the base change of Π to GL(4) over a CM extension E of F. Recall that, for certain algebraic Hecke characters χ of E, the twisted representation $\Pi_E(\chi)$ is conjugate self-dual. We consider the representations

$$\rho_{\pi,\iota,E} \overset{\text{df}}{=} \rho_{\Pi_E(\chi),\iota} \otimes \rho_{\check{\chi},\iota}.$$

Up to isomorphism, this is independent of χ. Indeed, for each place $w \nmid \ell$ of E,

$$\iota \mathrm{WD}(\rho_{\pi,\iota,E}|_{W_{E_w}})^{F-ss} \simeq \mathrm{rec}_4(\Pi_{E,w} \otimes |\det|^{-\frac{3}{2}}).$$

We only consider CM extensions E, in which v_0 splits, such that Π_E is cuspidal. Here v_0 is the place of F where π_{v_0} is of Steinberg type. This collection $\mathcal{I}$ is certainly strongly $\varnothing$-general, according to the example in the previous section. Moreover, the family of 4-dimensional Galois representations $\rho_{\pi,\iota,E}$ satisfies the patching conditions (a) and (b). For example, to check the *Galois invariance*,

$$\rho^{\theta}_{\pi,\iota,E} \simeq \rho_{\Pi_E(\chi)^{\theta},\iota} \otimes \rho_{\check{\chi}^{\theta},\iota} \simeq \rho_{\Pi_E(\chi)^{\vee},\iota} \otimes \rho_{\check{\chi}^{\theta},\iota} \simeq \rho_{\Pi_E(\chi^{\theta}),\iota} \otimes \rho_{\check{\chi}^{\theta},\iota},$$

by our choice of χ. Taking χ^{θ} instead of χ, then shows that $\rho^{\theta}_{\pi,\iota,E}$ is isomorphic to $\rho_{\pi,\iota,E}$ by the aforementioned independence. Alternatively, one can use the local description of $\rho_{\pi,\iota,E}$ above at the unramified places, and the fact that Π_E is a base change from F. To check the *compatibility*, note that for $w \nmid \ell$,

$$\iota \mathrm{WD}(\rho_{\pi,\iota,E}|_{W_{(EE')_w}})^{F-ss} \simeq \mathrm{rec}_4(\Pi_{v,(EE')_w} \otimes |\det|^{-\frac{3}{2}}),$$

and similarly for $\rho_{\pi,\iota,E'}$. See Lemma VII.2.6 in [HT]. Now (b) follows from Cebotarev. By the patching lemma, we finally get a continuous representation

$$\rho_{\pi,\iota} : \Gamma_F \to \mathrm{GL}_4(\bar{\mathbb{Q}}_\ell), \quad \rho_{\pi,\iota}|_{\Gamma_E} \otimes \rho_{\chi,\iota} \simeq \rho_{\Pi_E(\chi),\iota}.$$

It is *irreducible*, since $\rho_{\Pi_E(\chi),\iota}$ is known to be irreducible [TY], and satisfies:

$$\iota \mathrm{WD}(\rho_{\pi,\iota}|_{W_{F_v}})^{F-ss} \simeq \mathrm{rec}_{\mathrm{GT}}(\pi_v \otimes |c|^{-\frac{3}{2}}),$$

at each finite place $v \nmid \ell$ of F. Here $\mathrm{rec}_{\mathrm{GT}}$ is the local Langlands correspondence for GSp(4), as defined by Gan and Takeda in [GT]. To see this, pick any E in which v splits, and use the local description of $\rho_{\pi,\iota,E}$ together with the fact that Π is a *strong* lift of π. From the list of properties of $\rho_{\Pi_E(\chi),\iota}$, we then read off:

- Let $v \nmid \ell$ be a finite place of F, and let α be an eigenvalue of $\rho_{\pi,\iota}(\sigma)$ for some $\sigma \in W_{F_v}$. Then α belongs to $\bar{\mathbb{Q}}$, and for every embedding $\bar{\mathbb{Q}} \hookrightarrow \mathbb{C}$,
$$|\alpha| \in q_v^{\frac{\mathbb{Z}}{2}}.$$
- Let $v \nmid \ell$ be a finite place, with π_v *unramified*, and let α be an eigenvalue of $\rho_{\pi,\iota}(\mathrm{Frob}_v)$. Then α belongs to $\bar{\mathbb{Q}}$, and for every embedding $\bar{\mathbb{Q}} \hookrightarrow \mathbb{C}$,
$$|\alpha| = q_v^{\frac{w+3}{2}}.$$
- The representation $\rho_{\pi,\iota}$ is potentially semistable at any finite place $v|\ell$. Moreover, $\rho_{\pi,\iota}$ is crystalline at a finite place $v|\ell$ when π_v is unramified.

For the second part, we recall that χ is an algebraic Hecke character with infinity types $z^a\bar{z}^b$, where $a+b=w$. In particular, for the *unitary* twist π° we have:
$$L_v(s-\frac{1}{2}(w+3),\pi^\circ,\mathrm{spin}) = \det(1-\iota\rho_{\pi,\iota}(\mathrm{Frob}_v)\cdot q_v^{-s})^{-1}$$
at all places $v \nmid \ell$ where π° is unramified. Note that, by twisting $\rho_{\pi,\iota}$ with integral powers of the cyclotomic character χ_{cyc}, we may alter the motivic weight $w+3$ by any even integer. We compare with the motivic weight k_1+k_2-3 in [Wei].

Temperedness of π°*:* From the above, it follows immediately that π° has unitary Satake parameters at all places $v \nmid \ell$ where π° is unramified. In fact, π° is tempered at *every* place v: Indeed, by Corollary VII.1.11 in [HT], we know that Π_E is essentially tempered everywhere. That is, $\phi_{\pi_v}|_{W_{E_w}}$ has bounded image in $\mathrm{GL}_4(\mathbb{C})$ for every finite place w of E. Consequently, the same holds for $\phi_{\pi_v}|_{W_{F_v}}$.

The image of $\rho_{\pi,\iota}$*:* Since the eigenvalues of $\rho_{\pi,\iota}(\mathrm{Frob}_v)$ coincide with the integral Satake parameters of π_v, for finite $v \nmid \ell$ where π_v is unramified, Cebotarev yields:
$$\rho_{\pi,\iota}^\vee \simeq \rho_{\pi,\iota}\otimes\chi^{-1}, \quad \chi \overset{\mathrm{df}}{=} \omega_{\pi^\circ}\cdot\chi_{\mathrm{cyc}}^{-w-3},$$
where we confuse ω_{π° with its finite order ℓ-adic avatar. In other words, the space of $\rho_{\pi,\iota}$ has a non-degenerate bilinear form preserved by Γ_F with similitude χ. We have already observed that $\rho_{\pi,\iota}$ is irreducible, so by Schur's lemma this bilinear form must be symmetric *or* symplectic. Thus, the image of $\rho_{\pi,\iota}$ can always be conjugated into $\mathrm{GO}(4)$ or $\mathrm{GSp}(4)$. Under our running assumptions on π, in fact into the latter: Otherwise, by local-global compatibility at the place $v_0 \nmid \ell$, the L-parameter of Π_{v_0} is of orthogonal type. That is, it maps
$$\mathrm{rec}(\Pi_{v_0}) : W'_{F_{v_0}} = W_{F_{v_0}}\times\mathrm{SL}(2,\mathbb{C}) \to \mathrm{GO}(4,\mathbb{C}).$$
However, Π_{v_0} is the transfer of π_{v_0}, so $\mathrm{rec}(\Pi_{v_0})$ also preserves a symplectic form on $\mathbb{C}^4$. Now, Π_{v_0} is a generalized Steinberg representation, and one verifies that
$$Z_{\mathrm{GL}(4,\mathbb{C})}(\mathrm{im}(\mathrm{rec}(\Pi_{v_0}))) = \mathbb{C}^*$$

by an easy computation. Indeed, $\mathrm{rec}(\Pi_{v_0})$ is of the form $\phi \boxtimes S_d$, where ϕ is an irreducible representation of $W_{F_{v_0}}$, and S_d is the d-dimensional irreducible representation of $\mathrm{SL}(2,\mathbb{C})$. Ergo, the above symplectic form must agree with the orthogonal form up to a scalar. This is a contradiction. The symplecticity of $\rho_{\pi,\iota}$, just shown, is a special case of Theorem F on p. 6 in [CCl] when ω_π is trivial. This result from [CCl] has recently been generalized to the CM case in [BCh]. When $F=\mathbb{Q}$, the symplecticity of $\rho_{\pi,\iota}$ is shown in [Wei], for globally generic π, using Poincare duality. Indeed, by [Sou], π occurs with multiplicity one, so $\rho_{\pi,\iota}$ can be realized as the π_f-isotypic component of H^3 of a Siegel threefold. The cup product pairing then provides the desired symplectic form.

Baire category theory: To check that the image of $\rho_{\pi,\iota}$ is in fact contained in $\mathrm{GSp}_4(L)$, for some finite extension L over $\mathbb{Q}_\ell$, we invoke the Baire Category Theorem: Every locally compact Hausdorff space is a Baire space (that is, the union of any countable collection of closed sets with empty interior has empty interior). We will apply it to the compact subgroup $\rho_{\pi,\iota}(\Gamma_F)$ inside $\mathrm{GSp}_4(\bar{\mathbb{Q}}_\ell)$.

$$\rho_{\pi,\iota}(\Gamma_F)=\bigcup\nolimits_{L/\mathbb{Q}_\ell \text{ finite}}\rho_{\pi,\iota}(\Gamma_F)\cap \mathrm{GSp}_4(L)$$

is a countable union of closed subgroups, since each L is complete. Therefore,

$$\rho_{\pi,\iota}(\Gamma_F)\cap \mathrm{GSp}_4(L) \text{ has } \textit{non-empty} \text{ interior},$$

for some L, and hence this is an open subgroup. That is, the image of Γ_M for some finite extension M over F. In particular, it has *finite* index in $\rho_{\pi,\iota}(\Gamma_F)$. By enlarging L, to accomodate the finitely many coset representatives, we can arrange for the image of $\rho_{\pi,\iota}$ to be contained in the L-rational points $\mathrm{GSp}_4(L)$.

Total oddness: $\chi(c)=-1$ for every complex conjugation $c\in\Gamma_F$ from $\bar{\mathbb{Q}}\hookrightarrow\mathbb{C}$.

Hodge-Tate weights: Let us fix an embedding $s: F\to\bar{\mathbb{Q}}_\ell$, and let v be the associated place of F above ℓ. We wish to compute the Hodge-Tate weights of $\rho_{\pi,\iota}$ restricted to Γ_{F_v}, where $F_v=s(F)^-$. That is, for each integer j, evaluate

$$\dim_{\bar{\mathbb{Q}}_\ell}\mathrm{gr}^j(\rho_{\pi,\iota}\otimes_{F_v}B_{dR})^{\Gamma_{F_v}}.$$

We will reduce this to the analogous result for $\rho_{\Pi_E(\chi),\iota}$ already mentioned. Thus, we fix a CM extension E, in which v splits. Once and for all, we fix a divisor w of v, and look at a corresponding embedding $\tilde{s}: E\to\bar{\mathbb{Q}}_\ell$ over s. This canonically identifies $E_w=\tilde{s}(E)^-$ with F_v. Now note that, for characters χ as above,

$$\rho_{\pi,\iota}|_{\Gamma_{F_v}}\otimes\rho_{\chi,\iota}|_{\Gamma_{E_w}}\simeq\rho_{\Pi_E(\chi),\iota}|_{\Gamma_{E_w}}.$$

Therefore, we first record the Hodge-Tate weight of $\rho_{\chi,\iota}|_{\Gamma_{E_w}}$. The associated complex embedding $\iota(\tilde{s})$ defines an infinite place of E, where χ has the form $z^a\bar{z}^b$. As is well documented elsewhere in the literature, for example in [Bla], the Hodge-Tate weight is then $-b$, with our choice of normalization. Therefore,

$$\dim_{\bar{\mathbb{Q}}_\ell}\mathrm{gr}^j(\rho_{\pi,\iota}\otimes_{F_v}B_{dR})^{\Gamma_{F_v}}=\dim_{\bar{\mathbb{Q}}_\ell}\mathrm{gr}^{j-b}(\rho_{\Pi_E(\chi),\iota}\otimes_{E_w}B_{dR})^{\Gamma_{E_w}},$$

since D_{dR} is a $\otimes$-functor. It remains to find the highest weight of the $\mathcal{V}$ with

$$H^\bullet(\mathfrak{g}, K; \Pi_E(\chi)_\infty \otimes \mathcal{V}^*) \neq 0.$$

More precisely, we let $\sigma = \iota(s) \in \Sigma$, and consider the two complex embeddings $\{\tilde{\sigma}, \tilde{\sigma}^c\}$ of E extending σ. Here $\tilde{\sigma} = \iota(\tilde{s})$. In our earlier notation, we need to compute the quadruple $\mu(\tilde{\sigma}^c)$. For this, we follow the proof of Lemma 3.14 on p. 114 in [Cl2]: We consider the local component of $\Pi_E(\chi)$ at the infinite place of E above σ. We know its L-parameter, so according to p. 113 in [Cl2]:

$$\begin{cases} \mu_1(\tilde{\sigma}^c) = b + 3 - \frac{1}{2}(\mathbf{w} + n'), \\ \mu_2(\tilde{\sigma}^c) = b + 2 - \frac{1}{2}(\mathbf{w} + n), \\ \mu_3(\tilde{\sigma}^c) = b + 1 - \frac{1}{2}(\mathbf{w} - n), \\ \mu_4(\tilde{\sigma}^c) = b + 0 - \frac{1}{2}(\mathbf{w} - n'). \end{cases}$$

Here we have introduced $n = \nu_1 - \nu_2$ and $n' = \nu_1 + \nu_2$. Moreover, the motivic weight $w + 3$ is denoted by $\mathbf{w}$. From the above, and the result from section 4.2, we deduce that the Hodge-Tate weights of $\rho_{\pi,\iota}|_{\Gamma_{F_v}}$ are given by the sequence:

$$\frac{1}{2}(\mathbf{w} - n') < \frac{1}{2}(\mathbf{w} - n) < \frac{1}{2}(\mathbf{w} + n) < \frac{1}{2}(\mathbf{w} + n').$$

In particular, they are distinct. We will rewrite this slightly. For each $\sigma \in \Sigma$,

$$\delta = \delta(\sigma) \stackrel{\text{df}}{=} \frac{1}{2}(\mathbf{w} - n') = \frac{1}{2}(w - \mu_1 - \mu_2) \in \mathbb{Z}.$$

With this notation, the set of Hodge-Tate weights takes the following form:

$$\mathrm{HT}(\rho_{\pi,\iota}|_{\Gamma_{F_v}}) = \{\delta, \nu_2 + \delta, \nu_1 + \delta, \nu_1 + \nu_2 + \delta\}.$$

In the case $F = \mathbb{Q}$ it is customary to take $\mathbf{w} = k_1 + k_2 - 3$, that is, $\delta = 0$. In this case, we recover the Hodge types given in Theorem III on p. 2 in [Wei].

4.5 Consequences of local-global compatibility

Parahoric subgroups: We fix a finite place v of F, and define certain compact open subgroups of $\mathrm{GSp}_4(F_v)$, known as the parahoric subgroups. They arise as stabilizers of points in the Bruhat-Tits builidng. We refer to [Tit] for a general discussion. First, we have the *hyperspecial* maximal compact subgroup

$$K = K_v \stackrel{\text{df}}{=} \mathrm{GSp}_4(\mathcal{O}_v).$$

Inside of it, we have the pullbacks of the two parabolics via the reduction map:

$$\begin{cases} J_P = J_{P,v} \stackrel{\text{df}}{=} \{k \in K \colon k \pmod{v} \in P(\mathbb{F}_v)\}, \\ J_Q = J_{Q,v} \stackrel{\text{df}}{=} \{k \in K \colon k \pmod{v} \in Q(\mathbb{F}_v)\}. \end{cases}$$

They are usually called the *Siegel* and *Klingen* parahoric, respectively. Moreover,

$$I = I_v \stackrel{\text{df}}{=} J_P \cap J_Q = \{k \in K\colon\ k \pmod v \in B(\mathbb{F}_v)\}$$

is called the (upper-triangular) *Iwahori* subgroup. Furthermore, let us introduce

$$\eta = \eta_v \stackrel{\text{df}}{=} \begin{pmatrix} & & 1 & \\ & & & 1 \\ \varpi_v & & & \\ & \varpi_v & & \end{pmatrix}, \quad c(\eta) = -\varpi_v, \quad \eta^2 = \varpi_v \cdot I_4.$$

This η is occasionally referred to as the *Atkin-Lehner* element. It depends on the choice of a uniformizer ϖ_v, but it is well-defined modulo the maximal compact subgroup of the torus T_c. An explicit calculation shows that the η-conjugate $\eta K \eta^{-1}$ is another hyperspecial maximal compact subgroup containing the Siegel parahoric. There is one more maximal compact subgroup containing I. Namely,

$$\tilde{K} = \tilde{K}_v \stackrel{\text{df}}{=} \text{subgroup generated by } J_Q \text{ and its } \eta\text{-conjugate}.$$

This is the *paramodular*, or non-special, subgroup. We have thus described all parahoric subgroups of $\mathrm{GSp}_4(F_v)$ up to conjugacy. Note that η normalizes $\tilde{K}$ and J_P, hence I. Therefore, if J is any one of these subgroups, and π is an irreducible admissible representation, $\pi(\eta)$ is a well-defined operator on the J-invariants π^J. Its square is multplication by $\omega_\pi(\varpi_v)$. In particular, if $\omega_\pi = 1$, the eigenvalues of $\pi(\eta)$ are ± 1. These are tabulated in table 3 on p. 16 in [Sch].

Nilpotent orbits: Suppose π is an irreducible representation of $\mathrm{GSp}_4(F_v)$, assumed to be Iwahori-spherical. That is, $\pi^I \neq 0$. Then its L-parameter is given by a semisimple element in $\mathrm{GSp}_4(\mathbb{C})$ plus a compatible nilpotent element N in the Lie algebra $\mathfrak{gsp}_4(\mathbb{C})$, both viewed up to conjugacy. Here we list the finitely many possibilities for N. First, by the theory of the Jordan normal form,

$$\begin{pmatrix} 0 & 1 & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & & \\ & 0 & & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & 0 & \\ & & & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & 0 & 1 \\ & & & 0 \end{pmatrix}$$

represent the non-trivial nilpotent classes in $\mathfrak{gl}_4(\mathbb{C})$. An explicit computation verifies that the third representative *cannot* be conjugated into $\mathfrak{gsp}_4(\mathbb{C})$. Recall that $\mathfrak{sp}_4(\mathbb{C})$ consists of X such that JX is symmetric. Here J is the anti-diagonal symplectic form fixed throughout the paper. However, the other three representatives *are* in fact symplectic in this sense: They are conjugate to

$$\mathcal{N}_1 \stackrel{\text{df}}{=} \begin{pmatrix} 0 & & & \\ & 0 & 1 & \\ & & 0 & \\ & & & 0 \end{pmatrix}, \mathcal{N}_2 \stackrel{\text{df}}{=} \begin{pmatrix} 0 & 1 & & \\ & 0 & & \\ & & 0 & -1 \\ & & & 0 \end{pmatrix}, \mathcal{N}_3 \stackrel{\text{df}}{=} \begin{pmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & 0 & -1 \\ & & & 0 \end{pmatrix}$$

respectively. Again, this follows immediately from the theory of normal forms. Each $\mathcal{N}_i$ is contained in $\mathfrak{sp}_4(\mathbb{C})$. Note that $\mathcal{N}_i$ has rank i. It may be useful to observe that $\mathcal{N}_1$ is a root vector for the *long* simple root $\beta(t) = 2t_2$, whereas $\mathcal{N}_2$ is a root vector for the *short* simple root $\alpha(t) = t_1 - t_2$. Their sum is $\mathcal{N}_3$. By the Jacobson-Morozov theorem, [Jac, Theorem 3], the $\mathcal{N}_i$ in fact represent the $\mathrm{GSp}_4(\mathbb{C})$-conjugacy classes of nilpotent elements in $\mathfrak{gsp}_4(\mathbb{C})$. To aid comparison with [Sch], let us make the following remark: For the L-parameter of π to have a more transparent semisimple part, one often takes a different set of representatives, see p. 6 in [Sch]. For example, the two nilpotent elements

$$\mathcal{N}_1' \overset{\text{df}}{=} \begin{pmatrix} 0 & & & 1 \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{pmatrix}, \quad \mathcal{N}_2' \overset{\text{df}}{=} \begin{pmatrix} 0 & & & 1 \\ & 0 & 1 & \\ & & 0 & \\ & & & 0 \end{pmatrix},$$

are $\mathrm{GSp}_4(\mathbb{C})$-conjugate to $\mathcal{N}_1$ and $\mathcal{N}_2$ respectively. This is easy to check.

Iwahori-spherical generic representations: By a well-known result of Casselman, see [Car] for a nice review, the Iwahori-spherical π are precisely the constituents of unramified principal series. The way they decompose, in the case of GSp_4, was written out explicitly in [ST]. One gets 17 families of representations,

$$I, \; IIa, \; IIb, \; IIIa, \; IIIb, \; IVa - IVd, \; Va - Vd, \; VIa - VId,$$

according to how the unramified principal series breaks up. We refer to pages 6-8 in [Sch] for a precise definition of each class of representations. Fortunately, here we are only interested in the *generic* representations. That is, the 6 classes

$$I, \; IIa, \; IIIa, \; IVa, \; Va, \; VIa.$$

We will briefly recall the definition of each of these classes. To do that, we will first introduce the notation used in [ST]: For three quasi-characters χ_i, let

$$\chi_1 \times \chi_2 \rtimes \chi_3 \overset{\text{df}}{=} \mathrm{Ind}_B(\chi_1 \otimes \chi_2 \otimes \chi_3)$$

be the principal series for GSp_4 obtained by normalized induction from

$$\chi_1 \otimes \chi_2 \otimes \chi_3 : t \mapsto \chi_1(t_1)\chi_2(t_2)\chi_3(c(t)).$$

Similarly, if τ is an irreducible representation of GL_2, and χ is a character, let

$$\tau \rtimes \chi \overset{\text{df}}{=} \mathrm{Ind}_P(\tau \otimes \chi), \quad \chi \rtimes \tau \overset{\text{df}}{=} \mathrm{Ind}_Q(\chi \otimes \tau).$$

Again, we use *normalized* induction, and we identify the Levi subgroups of P and Q with $\mathrm{GL}_2 \times \mathrm{GL}_1$ in the natural way. Having this notation at hand, we describe the generic classes of Iwahori-spherical representations discussed above:

$$(I)\ \pi=\chi_1\times\chi_2\rtimes\chi_3,$$

$$(IIa)\ \pi=\mathrm{St}_{\mathrm{GL}(2)}(\chi_1)\rtimes\chi_2,$$

$$(IIIa)\ \pi=\chi_1\rtimes\mathrm{St}_{\mathrm{GL}(2)}(\chi_2),$$

$$(IVa)\ \pi=\mathrm{St}_{\mathrm{GSp}(4)}(\chi),$$

$$(Va)\ \pi\subset\mathrm{St}_{\mathrm{GL}(2)}(\nu^{1/2}\xi_0)\rtimes\nu^{-1/2}\chi$$

$$(VIa)\ \pi\subset\mathbf{1}\rtimes\mathrm{St}_{\mathrm{GL}(2)}(\chi)$$

Here all the characters χ and χ_i are unramified. Moreover, ν denotes the normalized absolute value, and ξ_0 is the non-trivial unramified quadratic character. According to Table 1 on p. 9 in [Sch], only IVa and Va are discrete series. Type VIa representations are the analogues of *limits* of discrete series. Table 3 on p. 16 in [Sch] lists the dimensions of the parahoric fixed spaces for all 17 families above, plus additional data such as the Atkin-Lehner eigenvalues when $\omega_\pi=1$. Below, we concatenate parts of Table 2 and parts of Table 3 in [Sch]. That is,

type	N	K	$\tilde{K}$	J_P	J_Q	I
I	0	1	2	4	4	8
IIa	$\mathcal{N}_1$	0	1	1	2	4
$IIIa$	$\mathcal{N}_2$	0	0	2	1	4
IVa	$\mathcal{N}_3$	0	0	0	0	1
Va	$\mathcal{N}_2$	0	0	0	1	2
VIa	$\mathcal{N}_2$	0	0	1	1	3

Table A: Parahoric fixed spaces and monodromy

We note that the assignment of monodromy operators in [Sch] is compatible with the local Langlands correspondence, as defined by Gan and Takeda via theta correspondence. This follows from the explicit calculations in section 12 of [GT], see their remarks on p. 33. By local-global compatibility, we deduce:

Corollary 1. *Let $\rho_{\pi,\iota}$ be the Galois representation attached to a globally generic cusp form π as above. Let $v\nmid\ell$ be a finite place of F such that π_v is Iwahori-spherical and ramified. Then $\rho_{\pi,\iota}|_{I_{F_v}}$ acts unipotently. In fact, the image $\rho_{\pi,\iota}(I_{F_v})$ is topologically generated by a $GSp_4(\bar{\mathbb{Q}}_\ell)$-conjugate of $\exp(\mathcal{N}_i)$, where*

$$i=\begin{cases}1, & \pi_v \text{ of type IIa},\\ 2, & \pi_v \text{ of type IIIa, Va, or VIa},\\ 3, & \pi_v \text{ of type IVa}.\end{cases}$$

In particular, we have the following consequences conjectured in [GTi] and [SU]:

- *π_v of Steinberg type $\Longleftrightarrow$ monodromy has rank 3.*

- π_v *has a unique* J_Q*-fixed line* $\Longleftrightarrow$ *monodromy has rank* 2.
- π_v *para-spherical* $\Longleftrightarrow$ *monodromy has rank* 1.

Proof. This follows immediately from Table A above. □

The first two consequences are part of the Conjecture on p. 11 in [GTi]. Note that part 4 of that Conjecture is false: If π_v has a unique J_P-fixed line, one cannot deduce that monodromy has rank one. The last consequence is Conjecture 3.1.7 on p. 41 in [SU], for globally generic π as above. Skinner and Urban used the holomorphic analogue as a substitute for deep results of Kato, in order to study Selmer groups for certain modular forms of square-free level. Another application to the Bloch-Kato conjecture in this context, contingent on the holomorphic analogue of the third consequence above, was given in [Sor].

Supercuspidal generic representations: According to Table 2 on p. 51 in [GT], there are two types of supercuspidal generic representations π of GSp_4. Firstly,

$$\pi = \theta((\sigma \otimes \sigma')^+),$$

for distinct supercuspidal representations $\sigma \neq \sigma'$ on GL_2. In this case, the lift to GL_4 is the isobaric sum $\sigma \boxplus \sigma'$. Secondly, if π is not a lift from $\mathrm{GO}_{2,2}$, when lifted to GL_4 it remains supercuspidal. Again, by local-global compatibility:

Corollary 2. *Let $\rho_{\pi,\iota}$ be the Galois representation attached to a globally generic cusp form π as above. Let $v \nmid \ell$ be a finite place of F such that π_v is supercuspidal. Then $\rho_{\pi,\iota}$ is trivial on some finite index subgroup of I_{F_v}. Moreover,*

$$\pi_v \text{ is } \underline{\text{not}} \text{ a lift from } GO_{2,2} \Longleftrightarrow \rho_{\pi,\iota}|_{W_{F_v}} \text{ is irreducible.}$$

On the contrary, when π_v $\underline{\text{is}}$ a lift from $GO_{2,2}$, the restriction $\rho_{\pi,\iota}|_{W_{F_v}}^{ss}$ breaks up as a sum of two non-isomorphic irreducible two-dimensional representations.

Proof. This follows from the foregoing discussion. □

For a moment, let us continue with the setup of the previous Corollary. The exponent of the Artin conductor of $\rho_{\pi,\iota}|_{I_{F_v}}$ is defined by the standard formula:

$$\mathfrak{f}(\rho_{\pi,\iota}|_{I_{F_v}}) \overset{\text{df}}{=} \sum_{i=0}^{\infty} \frac{1}{[\tilde{I}_{F_v} : \tilde{I}_{F_v,i}]} \cdot \operatorname{codim}_{\bar{\mathbb{Q}}_\ell}(\rho_{\pi,\iota}^{\tilde{I}_{F_v,i}}) \in \mathbb{Z},$$

where $\tilde{I}_{F_v,i}$ is the ith ramification group in $\tilde{I}_{F_v}$, in turn some finite quotient of I_{F_v} through which $\rho_{\pi,\iota}$ factors. This sum is finite. The exponent of the Swan conductor, $\mathfrak{f}_{\mathrm{Swan}}$, is given by the same formula except the summation starts at $i = 1$. By irreducibility, it is easy to see that $\rho_{\pi,\iota}$ has no nonzero I_{F_v}-invariants:

$$\mathfrak{f}_{\mathrm{Swan}}(\rho_{\pi,\iota}|_{I_{F_v}}) = \mathfrak{f}(\rho_{\pi,\iota}|_{I_{F_v}}) - 4.$$

We wish to relate this to the *depth* of π_v, a non-negative rational number measuring its wild ramification. We very briefly recall the definition: Let G be (the rational points of) a connected reductive group over F_v, and let x be a point on its extended Bruhat-Tits building [Tit]. Its stabilizer G_x is the corresponding parahoric subgroup. In [MP], Moy and G. Prasad defined an exhaustive descending filtration of G_x, consisting of open subgroups $G_{x,r}$ parametrized by non-negative real numbers r. They then defined a pro-p group G_{x,r^+} to be the union of the $G_{x,s}$ for $s > r$. The breaks r, where G_{x,r^+} is a proper subgroup of $G_{x,r}$, is known to form an unbounded discrete subset of $\mathbb{R}$. The depth of π is

$$\mathrm{depth}(\pi) \overset{\mathrm{df}}{=} \inf\{r\colon \pi^{G_{x,r^+}} \neq 0, \text{ some } x\} \in \mathbb{Q}.$$

Here π is any irreducible admissible representation of G. Our goal is to show:

Proposition 1. *Let $\rho_{\pi,\iota}$ be the Galois representation attached to a globally generic cusp form π as above. Let $v \nmid \ell$ be a finite place of F such that π_v is supercuspidal, and <u>not</u> a lift from $GO_{2,2}$. Then we have the following identity:*

$$\mathfrak{f}_{Swan}(\rho_{\pi,\iota}|_{I_{F_v}}) = 4 \cdot \mathit{depth}(\pi_v).$$

Proof. As is well-known, see [Tat], the Artin conductor fits into the ϵ-factor:

$$\epsilon(s, \iota\mathrm{WD}(\rho_{\pi,\iota}|_{W_{F_v}}), \psi) = \epsilon(0, \iota\mathrm{WD}(\rho_{\pi,\iota}|_{W_{F_v}}), \psi) \cdot q_v^{-s(\mathfrak{f}(\rho_{\pi,\iota}|_{I_{F_v}})+4n(\psi))}.$$

Here ψ is some fixed non-trivial character of F_v, and $n(\psi)$ is the largest n such that ψ is trivial on $\mathfrak{p}_v^{-n}$. Similarly, if Π_v is the supercuspidal lift of π_v to GL_4,

$$\epsilon(s, \Pi_v, \psi) = \epsilon(0, \Pi_v, \psi) \cdot q_v^{-s(\mathfrak{f}(\Pi_v)+4n(\psi))}.$$

Here $\mathfrak{f}(\Pi_v)$ is the standard conductor of Π_v, that is, the smallest f such that Π_v has nonzero vectors fixed by the subgroup consisting of elements in $\mathrm{GL}_4(\mathcal{O}_v)$ whose last row is congruent to $(0, \ldots, 0, 1)$ modulo $\mathfrak{p}_v^f$. Hence, we deduce that

$$\mathfrak{f}(\rho_{\pi,\iota}|_{I_{F_v}}) = \mathfrak{f}(\Pi_v),$$

since the local Langlands correspondence for GL_4 preserves ϵ-factors. The determinant twist can be ignored. Now, the key ingredient is the following formula due to Bushnell and Frölich [BF], which holds for supercuspidals on any GL_n,

$$\mathfrak{f}(\Pi_v) = n \cdot \mathrm{depth}(\Pi_v) + n, \quad n = 4.$$

We note, in passing, that this formula was generalized to the square integrable case in [LR]. It remains to explain why π_v and Π_v have the same depth. Keep in mind that $\Pi_v \otimes \omega_{\pi_v}$ is the theta lift of π_v to $\mathrm{GSO}_{3,3}$. Now invoke the main result from [Pan], suitably extended to incorporate similitudes. For this last step, Lemma 2.2 on p. 7 in [GT] is very useful. We omit the details. □

Tame ramification: In the previous Proposition, let us take π_v to have depth zero. In other words, π_v has nonzero vectors fixed by the pro-unipotent radical of some parahoric subgroup. In this special case, $\rho_{\pi,\iota}|_{I_{F_v}}$ factors through the tame quotient $I^t_{F_v}$, a pro-cyclic group of pro-order prime-to-p. More concretely, $\rho_{\pi,\iota}|_{I_{F_v}}$ is the direct sum of four ℓ-adic characters of I_{F_v}, of finite order prime-to-p. Below, we will state a related result, due to Genestier and Tilouine in the rational case. Let χ be any complex character of $\mathbb{F}_v^*$ and view it as a character

$$\chi : J_{Q,v} \to \mathrm{GL}(2, \mathbb{F}_v) \times \mathbb{F}_v^* \to \mathbb{F}_v^* \to \mathbb{C}^*,$$

where the second map is projection. If π is an irreducible admissible representation of GSp_4, we will be looking at the space $\pi^{J_Q,\chi}$ of vectors on which J_Q acts via the character χ. When $\chi \neq 1$, this is non-trivial only for principal series:

Lemma 3. *Let π be an irreducible generic representation of $GSp_4(F_v)$, and let χ be a non-trivial character of $\mathbb{F}_v^*$, viewed as a character of J_Q as above. Then $\pi^{J_Q,\chi}$ is nonzero if and only if π is a tamely ramified principal series of the form*

$$\pi = \tilde{\chi} \times (unram.) \rtimes (unram.),$$

for some extension $\tilde{\chi}$ of χ inflated to a tamely ramified character of $\mathcal{O}_v^*$.

Proof. First, let us assume $\pi^{J_Q,\chi}$ contains nonzero vectors. On such vectors, the Iwahori subgroup I acts via the character $\chi \otimes 1 \otimes 1$. By Roche's construction of types for principal series [Roc], see the formulation on p. 10 in [So2], we deduce that π must be a subquotient of a principal series representation of the form

$$\tilde{\chi} \times \chi_1 \rtimes \chi_2$$

as in the Lemma. That is, both χ_i are unramified, and $\tilde{\chi}$ extends χ. Our goal is to show that this principal series is necessarily irreducible. For that, we use the criterion from Theorem 7.9 in [Tad]. Since $\tilde{\chi}$ is ramified, the only way it could be reducible is if $\chi_1 = \nu^{\pm 1}$. Recall that ν denotes the normalized absolute value on F_v. For simplicity, let us assume that $\chi_1 = \nu$. The other case is taken care of by taking the dual. Then, by Lemmas 3.4 and 3.9 in [ST], there is a sequence

$$0 \to \tilde{\chi} \rtimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma) \to \tilde{\chi} \times \nu \rtimes \nu^{-1/2}\sigma \to \tilde{\chi} \rtimes \mathbf{1}_{\mathrm{GL}(2)}(\sigma) \to 0,$$

where we write χ_2 as $\nu^{-1/2}\sigma$. Both constituents are irreducible. However, the quotient is non-generic, so π must be the subrepresentation. It remains to check

$$(\tilde{\chi} \rtimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma))^{J_Q,\chi} = 0.$$

This is done by explicit calculation: We fix a complete set of representatives,

$$Q\backslash G/J_Q = \{1, s_1, s_1 s_2 s_1\}, \quad s_1 \overset{\text{df}}{=} \begin{pmatrix} & 1 & & \\ 1 & & & \\ & & & 1 \\ & & 1 & \end{pmatrix}, \quad s_2 \overset{\text{df}}{=} \begin{pmatrix} 1 & & & \\ & & 1 & \\ & -1 & & \\ & & & 1 \end{pmatrix}.$$

We are inducing from the Klingen parabolic, and an easy argument shows that the χ-vectors in the induced representation are given by the χ-vectors in the representation of the Levi subgroup. In our case, we get the three contributions:

- $(\tilde{\chi} \otimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma))^{Q \cap J_Q, \chi} = \tilde{\chi}^{\mathcal{O}^*, \chi} \otimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma)^{\mathrm{GL}_2(\mathcal{O})} = 0$,
- $(\tilde{\chi} \otimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma))^{Q \cap s_1 J_Q s_1, \chi} = \tilde{\chi}^{\mathcal{O}^*} \otimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma)^{I, \chi} = 0$,
- $(\tilde{\chi} \otimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma))^{Q \cap s_1 s_2 s_1 J_Q s_1 s_2^{-1} s_1, \chi} = \tilde{\chi}^{\mathcal{O}^*, \chi'} \otimes \mathrm{St}_{\mathrm{GL}(2)}(\sigma)^{\mathrm{GL}_2(\mathcal{O})} = 0$.

Here χ' is some irrelevant character. This proves the only if part of the Lemma. The converse is easier. Indeed, by the same observation, it suffices to check that

$$(\tilde{\chi} \otimes \chi_1 \otimes \chi_2)^{B \cap J_Q, \chi} = \tilde{\chi}^{\mathcal{O}^*, \chi} \otimes \chi_1^{\mathcal{O}^*} \otimes \chi_2^{\mathcal{O}^*} \neq 0,$$

as follows from our assumptions on these characters. This finishes the proof. $\square$

As a last application of local-global compatibility, in conjunction with the previous Lemma, we obtain the following result due to Genestier and Tilouine in the rational case $F = \mathbb{Q}$; compare to the second part of Theorem 2.2.5 in [GTi].

Corollary 3. *Let $\rho_{\pi,\iota}$ be the Galois representation attached to a globally generic cusp form π as above. Let $v \nmid \ell$ be a finite place of F such that $\pi_v^{J_Q,\chi}$ is* <u>*nonzero*</u> *for some* <u>*non-trivial*</u> *tamely ramified character χ of $\mathcal{O}_v^*$. It follows that*

$$\rho_{\pi,\iota}|_{I_{F_v}} = 1 \oplus 1 \oplus \chi \oplus \chi.$$

Here χ is the character of I_{F_v} obtained via local class field theory. Moreover, one can arrange for the two eigenspaces, for 1 and χ, to be totally isotropic.

Proof. The previous Lemma. See also (vi) of Proposition 12.15 in [GT]. $\square$

In [GTi], this result was proved by a careful study of the bad reduction of Siegel threefolds with Klingen level structure at v. The eigenspace polarization comes from the cohomology of each irreducible component of the special fiber.

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Arithmetic of a fake projective plane and related elliptic surfaces

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Abstract. The purpose of the present paper is to explain the fake projective plane constructed by J. H. Keum from the point of view of arithmetic ball quotients. Beside the ball quotient associated with the fake projective plane, we also analize two further naturally related ball quotients whose minimal desingularizations lead to two elliptic surfaces, one already considered by J. H. Keum as well as the one constructed by M. N. Ishida in terms of p-adic uniformization.

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1 Introduction

In 1954, F. Severi raised the question if every smooth complex algebraic surface homeomorphic to the projective plane $\mathbb{P}_2(\mathbb{C})$ is also isomorphic to $\mathbb{P}_2(\mathbb{C})$ as an algebraic variety. To that point, this was classically known to be true in dimension one, being equivalent to the statement that every compact Riemann surface of genus zero is isomorphic to $\mathbb{P}_1(\mathbb{C})$. F. Hirzebruch and K. Kodaira were able to show that in all odd dimensions $\mathbb{P}_n(\mathbb{C})$ is the only algebraic manifold in its homeomorphism class. But it took over 20 years until Severi's question could be positively answered. One obtains it as a consequence of S-T. Yau's famous results on the existence of Kähler-Einstein metrics on complex manifolds. Two years after Yau's results, in [Mum79], D. Mumford discussed the question, if there could exist algebraic surfaces which are not isomorphic to $\mathbb{P}_2(\mathbb{C})$, but which are topologically close to $\mathbb{P}_2(\mathbb{C})$, in the sense that they have same Betti numbers as $\mathbb{P}_2(\mathbb{C})$. Such surfaces are nowadays commonly called *fake projective planes*, see [BHPVdV04]. The following characterization of fake projective planes follows immediately from standard results in the theory of algebraic surfaces in combination with above mentioned Yau's result:

Lemma 1.1. *A smooth algebraic surface X is a fake projective plane if and only if $c_2(X) = 3$, $c_1^2(X) = 9$, $q(X) = p_g(X) = 0$, and $\mathrm{kod}(X) = 2$. In particular, the universal covering of X is isomorphic to the unit ball $\mathbb{B}_2 \subset \mathbb{C}^2$ and consequently*

$$X \cong \Gamma\backslash\mathbb{B}_2 \tag{1.1}$$

where Γ is a discrete, cocompact, and torsion free subgroup of $Aut(\mathbb{B}_2) \cong \mathrm{PSU}(2,1)$.

Here, $c_2(X)$ and $c_1^2(X)$ denote the two Chern numbers of X which are interpreted as the Euler number and the selfintersection number of the canonical divisor respectively, $q(X)$ is the irregularity, $p_g(X)$ the geometric genus, and $\mathrm{kod}(X)$ is the Kodaira dimension of X.

In the above mentioned work [Mum79], Mumford was also able to show the existence of fake projective planes, constructing an example. However, his construction is based on the theory of p-adic uniformization and his example is not presented in the form (1.1), as one naturally would expect. Moreover, his example is not even a complex surface, but a surface defined (apriori) over the field of 2-adic numbers $\overline{\mathbb{Q}}_2$. But, p-adic methods were for long time the only way for producing examples of fake projective planes, of which only fnitely many can exist, as pointed out by Mumford. Further examples of p-adic nature have been given by M. -N. Ishida and F. Kato ([IK98]), whereas the first complex geometric example seems to be the one constructed by J. H. Keum in [Keu06]. Motivated by the work of M. N. Ishida ([Ish88]), the author finds a fake projective plane as a degree 7 (ramified) cyclic covering of an explicitely given properly elliptic surface. Again, as all the examples before, Keum's example is not given as a ball quotient. The breakthrough in the study of fake projective planes came with the recent work of G. Prasad and S. Yeung, [PY07], where the authors succeeded to determine all fake projective planes. The main technical tool in their proof is a general volume formula developed by Prasad which is applied to the case of $\mathrm{SU}(2,1)$, and combined with the fact that the fundamental group of a fake projective plane is arithmetic. The resulting arithmetic groups are given rather explicitely in terms of Bruhat-Tits theory.

In the following paper we identify Keum's fake projective plane with a ball quotient $X_{\Gamma'} = \Gamma'\backslash\mathbb{B}_2$. In fact, this ball quotient appears in [PY07] (see [PY07], 5. 9, and there the examples associated with the pair (7,2)). However, in this paper we use a slightly modified approach to this quotient, motivated by [Kat], who identified Mumford's fake projective plane as a connected component of a certain Shimura variety. Moreover, Mumford's 2-adic example can be considered as a kind of a "2-adic completion" of a ball quotient. This ball quotient also appears in [PY07] and is also associated to the pair $(7,2)$ (in the sense of [PY07]), but this ball quotient is not isomorphic to $X_{\Gamma'}$ as remarked in [Keu08].

Let us briefly describe the approach. We start with an explicit division algebra D over $\mathbb{Q}$ with an involution of second kind ι_b, a particular maximal order $\mathcal{O}$, and we consider the arithmetic group $\Gamma = \Gamma_{\mathcal{O},b}$ consisting of all norm-1 elements in $\mathcal{O}$ which are unitary with respect to the hermitian form corresponding to ι_b. Now, $\Gamma^{'}$ appears as a principal congruence subgroup of index 7 in Γ. The explicit knowledge of Γ allows us to see particular elements of finite order in Γ and gives us the possibility to explain the elliptic surface appearing in [Keu06] from the point of view of ball quotients, namely as the minimal desingularization of quotient singularities of $X_\Gamma = \Gamma\backslash\mathbb{B}_2$. Passing to a particular group $\tilde{\Gamma}$ containing Γ with index 3, we identify the minimal desingularization of the ball quotient $X_{\tilde{\Gamma}}$ with the elliptic surface of Ishida ([Ish88]) which is originally given in terms of p-adic uniformization. We illustrate the situation in the following diagram:

$$\begin{array}{ccc} & & X_{\Gamma'} \\ & & \downarrow{\scriptstyle 7} \\ \widetilde{X_\Gamma} & \longrightarrow & X_\Gamma \\ \downarrow & & \downarrow{\scriptstyle 3} \\ \widetilde{X_{\tilde{\Gamma}}} & \longrightarrow & X_{\tilde{\Gamma}} \end{array}$$

There, the arrows indicate finite cyclic coverings of compact ball quotients with announced degree, $X_{\Gamma'}$ is a fake projective plane, X_Γ and $X_{\tilde{\Gamma}}$ are singular ball quotients, having only cyclic singularities and $\widetilde{X_\Gamma}, \widetilde{X_{\tilde{\Gamma}}}$ are the canonical resolutions of singularities and are both smooth minimal elliptic surfaces of Kodaira dimension one. Identifying $\widetilde{X_{\tilde{\Gamma}}}$ with Ishida's elliptic surface in [Ish88], we know the singular fibers of its elliptic fibration. Explicit knowledge of the finite covering $X_\Gamma \longrightarrow X_{\tilde{\Gamma}}$ gives the elliptic fibration of $\widetilde{X_\Gamma}$, already determined by Keum.

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2 Preliminiaries on arithmetic ball quotients

In this section, we discuss arithmetically defined groups which act properly discontinuously on a symmetric domain isomorphic to the two-dimensional complex unit ball and collect some basic properties of the corresponding locally symmetric spaces.

2.1 Arithmetic lattices

If H is a hermitian form over $\mathbb{C}$ in three variables with two negative and one positive eigenvalue, then we speak of a form with signature $(2,1)$. The set of positive definite lines

$$\mathbb{B}_H = \{[l] \in \mathbb{P}_2(\mathbb{C}) \mid H(l,l) > 0\} \subset \mathbb{P}_2(\mathbb{C}) \tag{2.1}$$

with respect to such a hermitian form H is isomorphic to the two dimensional complex unit ball $\mathbb{B}_2$. Alternatively, we can see $\mathbb{B}_H$ as the symmetric space $\mathbb{B}_H \cong \mathrm{SU}(H)/K_0$ associated with the Lie group $\mathrm{SU}(H)$, that is the group of isometries with respect to H of determinant 1, where K_0 is a maximal compact subgroup in $\mathrm{SU}(H)$. Every cocompact discrete and torsion free subgroup Γ of $\mathrm{SU}(H)$ acts properly discontinously on $\mathbb{B}_H$ as a group of linear fractional transformations, but not effectively in general. However, the image $\mathbb{P}\Gamma$ of Γ in $\mathrm{PSU}(H)$ acts effectively. The orbit space $X_\Gamma = \Gamma\backslash\mathbb{B}_H$ has a natural structure of a complex manifold, and even more: it has the structure of a smooth projective algebraic variety. Arithmetic subgroups of $\mathrm{SU}(H)$ provide a large natural class of discrete groups which act on $\mathbb{B}_H$. By the classification theory of forms of algebraic groups, all arithmetic groups which act on the ball can be constructed as follows:

Let F be a totally real number field and K/F a pure imaginary quadratic extension (CM extension) of K. Let A be a 9-dimensional central simple algebra over K and assume that on A exists an *involution of second kind*, i. e. an anti-automorphism $\iota : A \to A$ such that $\iota^2 = id$ and the restriction $\iota|_K$ is the complex conjugation $x \mapsto \overline{x} \in \mathrm{Gal}(K/F)$. In that case, using the Skolem-Noether theorem, we can always normalize ι in such a way that the extension $\iota_{\mathbb{C}}$ on $A \otimes \mathbb{C} \cong M_3(\mathbb{C})$ of ι is the hermitian conjugation, $\iota_{\mathbb{C}}(m) = \overline{m}^t$. In this case we say that ι is the *canonical involution of second kind*.

As a central simple algebra over a number field, A is a cyclic algebra

$$A = A(L,\sigma,\alpha) = L \oplus Lu \oplus Lu^2, \tag{2.2}$$

where L/K is an (cyclic) extension of number fields of degree 3, σ is a generator of $\mathrm{Gal}(L/K)$ and $u \in A$ satisfies $\alpha = u^3 \in K^*$, $au = ua^\sigma$ for all $a \in L$. This data already determine the isomorphy class of A. The structure of a division algebra is determined by the class of α in $K^*/N_{L/K}(L^*)$ by class field theory: A is a division algebra if and only if $\alpha \notin N_{L/K}(L^*)$, otherwise A is the matrix algebra $M_3(K)$. We note that L is a splitting field of A, i. e. $A \otimes L \cong M_3(L)$ and that we can embedd A in $M_3(L)$ if we put:

$$a \mapsto \begin{pmatrix} a & 0 & 0 \\ 0 & a^\sigma & 0 \\ 0 & 0 & a^{\sigma\sigma} \end{pmatrix} \text{ for } a \in L,\ u \mapsto \begin{pmatrix} 0 & 0 & \alpha \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{2.3}$$

and extend linearly to all A.

Consider again the canonical involution ι of second kind on A and let $b \in A$ be an ι-invariant element, i. e. an element with $b^\iota = b$. Then $\iota_b : a \mapsto b a^\iota b^{-1}$ defines a further involution of second kind. Let $\mathbf{A}^{(1)}$ denote the group of elements in A of reduced norm 1 considered as an algebraic group and let $\mathbf{G}_b = \{g \in \mathbf{A}^{(1)} \mid g g^{\iota_b} = 1\}$. Then, $\mathbf{G}_b$ is an algebraic group defined over F. Let us further assume that the matrix corresponding to b, obtained from the embedding $A \hookrightarrow M_3(\mathbb{C})$ induced by $id \in \mathrm{Hom}(F, \mathbb{C})$, represents a hermitian form of signature $(2,1)$, and for every $id \neq \tau \in \mathrm{Hom}(F, \mathbb{C})$ the induced matrix is a hermitian form of signature $(3,0)$. Then the group of real valued points $\mathbf{G}_b(\mathbb{R})$ is isomorphic to the product $\mathrm{SU}(2,1) \times \mathrm{SU}(3)^{[F:\mathbb{Q}]-1}$. Since $\mathrm{SU}(3)$ is compact, according to the Theorem of Borel and Harish-Chandra, every arithmetic subgroup of $\mathbf{G}_b(F)$ is a lattice in $\mathrm{SU}(2,1)$, i. e. a discrete subgroup of finite covolume and acts properly discontinuously on the ball. The arithmetic subgroups derived from the pair (A, ι_b) can be specified in terms of orders in A: Every such group is commensurable to a group

$$\Gamma_{\mathcal{O},b} = \{\gamma \in \mathcal{O} \mid \gamma\gamma^{\iota_b} = 1, \quad \mathrm{nr}(\gamma) = 1\},$$

where $\mathcal{O}$ is a ι_b-invariant order in A and $\mathrm{nr}(\cdot)$ denotes the reduced norm. For instance, take $A = M_3(K)$ and let $H \in M_3(K)$ be hermitian with the property that its signature is $(2,1)$ when considered as matrix over $\mathbb{C}$ and that the signature of all matrices obtained by applying non-trivial Galois automorphisms $\tau \in \mathrm{Gal}(F/\mathbb{Q})$ to the entries is $(3,0)$. $M_3(\mathfrak{o}_K)$ is definitively an order in $M_3(K)$ and the arithmetic group $\Gamma_H = \mathrm{SU}(H, \mathfrak{o}_K)$ is called the (full) *Picard modular group*. On the other hand, the arithmetic lattices constructed from the division algebras are generally called *arithmetic lattices of second kind*.

2.2 Invariants of arithmetic ball quotients

Keeping the notations from the last paragraph, let $\mathbf{G}_b$ be an algebraic group derived from a pair (A, ι_b) for which b satisfies the additional condition $\mathbf{G}_b(\mathbb{R}) \cong \mathrm{SU}(2,1) \times \mathrm{SU}(3)^{[F:\mathbb{Q}]-1}$. Let Γ be an arithmetic subgroup in $\mathbf{G}_b(F)$ and denote $X_\Gamma = \Gamma \backslash \mathbb{B}_2$ the corresponding locally symmetric space. Then, the Godement's compactness criterion implies that X_Γ is compact, except in the case where A is the matrix algebra over an imaginary quadratic field K. After a possible descent to a finite index normal subgroup, we can assume that Γ is torsion free and X_Γ is smooth. There is always a volume form μ on $\mathbb{B}_2$ such that the volume $\mathrm{vol}_\mu(\Gamma)$ of a fundamental domain of Γ is exactly the Euler number of X_Γ, when Γ is torsion free and cocompact. Under the assumption that the arithmetic group is so-called *principal arithmetic subgroup* this volume can be given explicitely by formulas involving exclusively data of arithmetical nature. A principal arithmetic group Λ is defined as $\Lambda = \mathbf{G}_b(F) \cap \prod_v P_v$, where $\{P_v\}$ is a collection of parahoric subgroups $P_v \subset \mathbf{G}_b(F_v)$ (v a non-archimedian place of F), such that $\prod_v P_v$ is open in the adelic group $\mathbf{G}_b(\mathbb{A}_F)$ (see [Pra89], 3. 4, or [BP89],1. 4. for details). Let us recall this formula for principal arithmetic subgroups of $\mathrm{SU}(2,1)$ established in [PY07] where the reader will find omitted details (see also [Pra89] and [BP89] for the general case). Let D_K and D_F

denote the absolute values of discriminants of the number fields K and F and $\zeta_F(\cdot)$ the Dedekind zeta function of F. For $Re(s) > 1$ a L-function is defined by $L(s, \chi_{K/F}) = \prod_v (1 - \chi_{K/F}(\mathfrak{p}_v) N(\mathfrak{p}_v)^{-s})^{-1}$ where v runs over all finite places of F, $\mathfrak{p}_v$ denotes the prime ideal of $\mathfrak{o}_F$ corresponding to v, $N(\mathfrak{p}_v) = |\mathfrak{o}_F/\mathfrak{p}_v|$ and $\chi_{K/F}(\cdot)$ is a character defined to be 1,-1 or 0 according to whether $\mathfrak{p}_v$ splits, remains prime or ramifies in K.

LEMMA 2.1 (see [PY07]). *Let $\Lambda \subset \mathbf{G}_b(F)$ be a principal arithmetic subgroup. Then*

$$\mathrm{vol}_\mu(\Lambda) = 3 \frac{D_K^{5/2}}{D_F} (16\pi^5)^{-[F:\mathbb{Q}]} \zeta_F(2) L(3, \chi_{K/F}) \mathcal{E}$$

where $\mathcal{E} = \prod_{v \in S} e(v)$ is a product running over a finite set S of non-archimedian places of F determined by the localization of Λ with rational numbers $e(v)$, given explicitely in [PY07] 2. 5.

The above formula not only gives the Euler number of a smooth ball quotient X_Γ, when Γ is torsion free finite index normal subgroup of a principal arithmetic Λ, but also other numerical invariants. Namely, by Hirzebruch's Proportionality Theorem, $c_1^2(X_\Gamma) = 3c_2(X_\Gamma)$ for any smooth and compact ball quotient. Consequently, the Noether formula implies for the Euler-Poincaré characteristic $\chi(X_\Gamma) := \chi(\mathcal{O}_{X_\Gamma})$ of the structure sheaf $\mathcal{O}_{X_\Gamma}$ (arithmetic genus): $\chi(X_\Gamma) = c_2(X_\Gamma)/3$. Similarly, the signature $\mathrm{sign}(X_\Gamma)$ equals to $c_2(X_\Gamma)/3$ by Hirzebruch's Signature Theorem. In general, the remaining Hodge numbers (irregularity and the geometric genus) are not immediately given. But, for a large class of arithmetic groups, namely congruence subgroups of second kind, i. e. those defined by congruences and contained in division algebras, there is a vanishing Theorem of Rogawski (see [BR00], Theorem 1), saying that for such groups $H^1(\Gamma, \mathbb{C})$ vanishes. Then it follows that the irregularity of the corresponding ball quotients vanishes, since we can identify the two cohomology groups $H^*(\Gamma)$ and $H^*(X_\Gamma)$.

3 CONSTRUCTION OF THE FAKE PROJECTIVE PLANE

Let $\zeta = \zeta_7 = \exp(2\pi i/7)$ and $L = \mathbb{Q}(\zeta)$. Then, L contains the quadratic subfield $K = \mathbb{Q}(\lambda) \cong \mathbb{Q}(\sqrt{-7})$ with $\lambda = \zeta + \zeta^2 + \zeta^4 = \frac{-1+\sqrt{-7}}{2}$. The automorphism $\sigma : \zeta \mapsto \zeta^2$ generates a subgroup of $\mathrm{Gal}(L/\mathbb{Q})$ of index 2 and leaves K invariant, therefore, $\langle\sigma\rangle = \mathrm{Gal}(L/K)$. We put $\alpha = \lambda/\overline{\lambda}$. As we have seen before (compare (2.2)), the triple (L, σ, α) defines a cyclic algebra $D = D(L, \sigma, \alpha)$ over K.

LEMMA 3.1. *The algebra D is a division algebra and has an involution of second kind. The assignement $a \mapsto \bar{a}$ for $a \in L$, $u \mapsto \bar{\alpha}u^2$ defines the canonical involution of second kind ι. Let $b = tr(\lambda) + \bar{\lambda}u + \bar{\lambda}u^2$. Then, the induced hermitian matrix H_b has the signature* $(2, 1)$.

Proof. The choice of α ensures that $\alpha \notin N_{L/K}(L^*)$ by Hilbert's Theorem 90. This proves the first statement. The remaining statements are proven in an elementary way, using the matrix representation of D given in (2.3). ☐

Hence, the algebraic group $\mathbf{G}_b$ is a $\mathbb{Q}$-form of the real group SU(2, 1). Now, we construct an arithmetic subgroup in $\mathbf{G}_b(\mathbb{Q})$ derived from a maximal order in D. For this let

$$\mathcal{O} = \mathfrak{o}_L \oplus \mathfrak{o}_L \bar{\lambda} u \oplus \mathfrak{o}_L \bar{\lambda} u^2. \tag{3.1}$$

Clearly, $\mathcal{O}$ is an order in D. Also one easily sees that $\mathcal{O}$ is invariant under the involution ι_b defined by b. We know even more:

Lemma 3.2. *$\mathcal{O}$ is a maximal order in D.*

Proof. $\mathcal{O}$ is maximal if and only if the localization $\mathcal{O}_v$ is maximal for every finite place v. Over a local field, any central simple algebra A_v contains (up to a conjugation) the unique maximal order $\mathcal{M}_v$ (see [Rei03]). Therefore the discriminant $d(\mathcal{M}_v)$ completely characterizes $\mathcal{M}_v$. The discriminant $d(\mathcal{O})$ is easily computed to be 2^6. Since $d(\mathcal{O}_v) = d(\mathcal{O})_v$, we immediately see that at all places v not dividing 2, $d(\mathcal{O}_v) = 1$. Exactly at those places D_v is the matrix algebra, since α is an unit there, and $\mathcal{O}_v$ is maximal by [Rei03], p. 185. At the two places λ and $\bar{\lambda}$ dividing 2, D_v is a division algebra. There $d(\mathcal{O}_v)$ is exactly the discriminant of the maximal order $\mathcal{M}_v$ ([Rei03], p. 151). □

Let

$$\Gamma_{\mathcal{O},b} = \mathbf{G}_b(\mathbb{Q}) \cap \mathcal{O} = \{\gamma \in \mathcal{O} \mid \gamma\gamma^{\iota_b} = 1,\ \mathrm{nr}(\gamma) = 1\} \tag{3.2}$$

be the arithmetic subgroup of $\mathbf{G}_b(\mathbb{Q})$ defined by $\mathcal{O}$. We shall summarize some properties of $\Gamma_{\mathcal{O},b}$:

Lemma 3.3. *$\Gamma_{\mathcal{O},b}$ is a principal arithmetic subgroup. Every torsion element in $\Gamma_{\mathcal{O},b}$ has the order 7. All such elements are conjugate in D.*

Proof. By definition, $\Gamma_{\mathcal{O},b}$ will be principal if at all finite places p of $\mathbb{Q}$ its localization is a parahoric subgroup of $\mathbf{G}_b(\mathbb{Q}_p)$. Since $\mathcal{O}$ is maximal, at all places $p \neq 2$ the localization $\Gamma^{[p]}_{\mathcal{O},b}$ is the special unitary group $\mathrm{SU}(H_b, \mathfrak{o}_p)$, where $\mathfrak{o}_p = \mathfrak{o}_K \otimes \mathbb{Q}_p$. Then by [Tit79], $\Gamma^{[p]}_{\mathcal{O},b}$ is maximal parahoric. Since 2 is split in K, there is a division algebra D_2 over $\mathbb{Q}_2$ such that $D \otimes \mathbb{Q}_2 = D_2 \oplus D_2^o$, where D_2^o denotes the opposite algebra to D_2. The projection to the first factor gives an isomorphism $\mathbf{G}_b(\mathbb{Q}_2) \cong D_2^{(1)}$, the group of elements of reduced norm 1 in D_2. Let $\mathcal{M}_2$ be the maximal order in D_2. Then $\Gamma^{[2]}_{\mathcal{O},b} = \mathcal{M}_2^{(1)}$. Again, by [Tit79], this is a maximal parahoric group. In order to prove the second statement let us consider an element τ of finite order in $\Gamma_{\mathcal{O},b}$. Let η be an eigenvalue of τ. Then η is a root of unity and $\mathbb{Q}(\eta)$ is a commutative subfield of D. Conversely, every cyclotomic subfield of D containing K gives rise to an element of finite order in D. Consequently, we have a bijection between the set of the conjugacy classes of elements of finite order in D and the cyclotomic fields $C \subset D$ which contain the center K of D. Since L is the only such field, only elements of order 7, 2 and 14 can occur. But since the reduced norm of -1 is -1 again, elements of order 2 don't belong to Γ. Thus, only elements of order 7 are possible. □

Let us now consider a particular congruence subgroup of $\Gamma_{\mathcal{O},b}$, namely the principal congruence subgroup

$$\Gamma_{\mathcal{O},b}(\lambda) = \{\gamma \in \Gamma_{\mathcal{O},b} \mid \gamma \equiv 1 \bmod \lambda\} \quad (3.3)$$

We have

Lemma 3.4. *$\Gamma_{\mathcal{O},b}(\lambda)$ is torsion free subgroup of index $[\Gamma_{\mathcal{O},b} : \Gamma_{\mathcal{O},b}(\lambda)]=7$.*

Proof. By Lemma 3.3 we have to show that $\Gamma_{\mathcal{O},b}(\lambda)$ contains no elements of order 7. Let γ be an element in $\Gamma_{\mathcal{O},b}(\lambda)$ of finite order k. The eigenvalues of the representing matrix m_γ of γ are k-th roots of unity. Let η be such an eigenvalue and $E = \mathbb{Q}(\eta)$. Then $E \cong L$ by arguments in the proof of Lemma 3.3. Since γ belongs to the congruence subgroup defined by λ, λ divides the coefficients of $m_\gamma - 1_3 \in M_3(E)$. Let x be an eigenvector of m_γ. Multiplying with an integer we can assume $x \in \mathfrak{o}_E^3$. Then $\lambda|(m_\gamma - 1_3)x = (\eta - 1)x$ from which follows that λ divides $\eta - 1$ in $\mathfrak{o}_E$. Taking the norms we have $N_{E/\mathbb{Q}}(\lambda)|N_{E/\mathbb{Q}}(\eta-1)|k$. This is not possible when assuming $k = 7$. Therefore, $\Gamma_{\mathcal{O},b}(\lambda)$ is torsion free. In order to compute the index, we make use of the strong approximation property which holds for $\mathbf{G}_b$. It allows us to express the index $[\Gamma_{\mathcal{O},b} : \Gamma_{\mathcal{O},b}(\mathfrak{a})]$ of an arbitrary principal congruence subgroup $\Gamma_{\mathcal{O},b}(\mathfrak{a})$ defined by some ideal $\mathfrak{a} = \prod \mathfrak{p}^{n_\mathfrak{p}}$ of $\mathfrak{o}_K$ as a product of local indices $\prod_{p|\mathfrak{a}}[\Gamma^{[p]}_{\mathcal{O},b} : \Gamma^{[p]}_{\mathcal{O},b}(\mathfrak{p}^{n_\mathfrak{p}})]$, where $p = \mathfrak{p} \cap \mathbb{Q}$. In the case in question, we have $[\Gamma_{\mathcal{O},b} : \Gamma_{\mathcal{O},b}(\lambda)] = [\Gamma^{[2]}_{\mathcal{O},b} : \Gamma^{[2]}_{\mathcal{O},b}(\lambda)]$. But in the proof of Lemma 3.3 we already determined the structure of the localizations of $\Gamma_{\mathcal{O},b}$: $\Gamma^{[2]}_{\mathcal{O},b} \cong \mathcal{M}_2^{(1)}$ and therefore $\Gamma^{[2]}_{\mathcal{O},b}(\lambda)$ is the congruence subgroup $\mathcal{M}_2^{(1)}(\pi_{D_2})$, where π_{D_2} is the uniformizing element of D_2. It follows from a Theorem of Riehm ([Rie70] Theorem 7, see also [PY07]) that $[\mathcal{M}_2^{(1)} : \mathcal{M}_2^{(1)}(\pi_{D_2})] = [\mathbb{F}^*_{2^3} : \mathbb{F}^*_2] = 7$. □

Let us in the following shortly write Γ for $\Gamma_{\mathcal{O},b}$ and Γ' for $\Gamma_{\mathcal{O},b}(\lambda)$. The main result of this section is

Theorem 3.5. *The ball quotient $X_{\Gamma'}$ is a fake projective plane.*

Proof. First we would like to compute the Euler number $c_2(X_{\Gamma'})$ of $X_{\Gamma'}$. Since Γ' is torsion free, $c_2(X_{\Gamma'}) = vol(\Gamma') = [\Gamma : \Gamma']vol_\mu(\Gamma) = 7vol_\mu(\Gamma)$. By Lemma 3.3 Γ is principal, so we can apply Lemma 2.1 in order to compute $vol_\mu(\Gamma)$. Well known is the value $\zeta_\mathbb{Q}(2) = \pi^2/6$. The other value $L(3, \chi_K) = -\frac{7}{8}\pi^3 7^{-5/2}$ is computed using functional equation and the explicit formula for generalized Bernoulli numbers. In the last step, we determine the local factors $\mathcal{E}$. Looking at [PY07], 2. 2. non trivial local factors $e(v)$ can only occur for $v = 2$ and $v = 7$. Sections 2. 4. and 2. 5. of [PY07] give $e(2) = 3$ and $e(7) = 1$ since the localizations of Γ are maximal parahoric. Altoghether we get $vol_\mu(\Gamma) = 3/7$ and $c_2(X_{\Gamma'}) = 3$. Proportionality Theorem gives $c_1^2(X_{\Gamma'}) = 9$. Rogawski's vanishing result implies $q(X_{\Gamma'}) = 0$. Then automatically $p_g(X_{\Gamma'}) = 0$. As a smooth compact ball quotient $X_{\Gamma'}$ is a surface of general type. By Lemma 1.1 $X_{\Gamma'}$ is a fake projective plane. □

4 Structure of X_Γ

Let the notations be as in the last section and in particular $\Gamma := \Gamma_{\mathcal{O},b}$, $\Gamma^{'} := \Gamma_{\mathcal{O},b}(\lambda)$, let in addition $\mathbb{B}$ denote the ball defined by (the matrix representation of) b. In this section we are interested in the structure of the ball quotient $X_\Gamma = \Gamma\backslash\mathbb{B}$ by the arithmetic group Γ. According to Lemma 3.3, the elements of finite order in D correspond to the 7-th roots of unity. Hence, all elements of finite order in Γ are conjugated to a power of $\zeta = \zeta_7$. The torsion element ζ doesn't belong to Γ, since b is not invariant under the operation $b \mapsto \zeta b \zeta^\iota$. But $\zeta c \zeta^\iota = c$ for $c = \zeta + \zeta^{-1}$, which is ι-invariant element of signature $(2,1)$. For this reason $Z = g^{-1}\zeta g$ is an element of order 7 in Γ, where $g \in D$ is chosen such that $gbg^{-1} = c$. Therefore X_Γ is isomorphic to the quotient $X_{\Gamma'}/\langle Z\rangle$ by the finite subgroup $\langle Z\rangle < \Gamma$. Let $\psi : X_{\Gamma'} \longrightarrow X_{\Gamma'}/\langle Z\rangle$ denote the canonical projection.

Proposition 4.1. *The branch locus of ψ consists of three isolated points Q_1,Q_2,Q_3. They are cyclic singularities of X_Γ, all of type $(7,3)$. Outside of Q_1,Q_2,Q_3, X_Γ is smooth. The minimal resolution of each singularity Q_i, $i = 1,2,3$, is a chain of three rational curves $E_{i,1}$, $E_{i,2}$, $E_{i,3}$ with selfintersections $(E_{i,1})^2 = -3$, $(E_{i,2})^2 = (E_{i,3})^2 = -2$ and $(E_{i,1} \cdot E_{i,2}) = (E_{i,2} \cdot E_{i,3}) = 1$, $(E_{i,1} \cdot E_{i,3}) = 0$ (Hirzebruch-Jung string of type $(-3)(-2)(-2)$).*

Proof. The branch locus of ψ doesn't depend explicitely on $\Gamma^{'}$ and is in fact the image of the fixed point set in $\mathbb{B}$ of non-trivial finite order elements in Γ under the canonical projection $\mathbb{B} \longrightarrow \Gamma\backslash\mathbb{B}$ coming from the ball. The number of its components is exactly the number of Γ-equivalence classes of elliptic fixed points in $\mathbb{B}$. By (2.3) the matrix representation m_ζ of ζ is just $m_\zeta = diag(\zeta,\zeta^2,\zeta^4)$. Only one (projectivized) eigenvector of m_ζ–namely e_1–lies in the ball defined by c and represents an elliptic fixed point. Let $x := g^{-1}e_1$ denote the corresponding fixed point in $\mathbb{B}$ of Z. Note that ζ can be embedded into D in three different ways, namely as ζ, ζ^σ or $\zeta^{\sigma\sigma}$. The two non-trivial embeddings give two further Γ-inequivalent fixed points x^σ and $x^{\sigma\sigma}$ in the same way as x is given. Let $Q_i \in X_\Gamma$, $i = 1,2,3$ be the images of x, x^σ, $x^{\sigma\sigma}$ under the canonical projection. They give the three branch points. It is left to show that there are no more such points and that there are no curves in the branch locus. We will give an argument for it subsequent to the next Proposition. Looking at the action of $\langle m_\zeta\rangle$ around e_1 we find that around Q_i $X_{\Gamma_{\mathcal{O},b}}$ looks like $\mathbb{C}^2/G$, with $G \cong \langle diag(\zeta,\zeta^3)$, which represents a cyclic singularity of type $(7,3)$. By standard methods we get the minimal resolution stated above.

Let $\widetilde{X_\Gamma} \xrightarrow{\rho} X_\Gamma$ denote the minimal resolution of all singularities of X_Γ. Our goal is to determine the structure of $\widetilde{X_\Gamma}$. We start with topological invariants.

Proposition 4.2. $c_2(\widetilde{X_\Gamma}) = 12$, $\operatorname{sign}(\widetilde{X_\Gamma}) = -8$. *Consequently* $c_1^2(\widetilde{X_\Gamma}) = 0$, $\chi(\widetilde{X_\Gamma}) = 1$.

Proof. In [Hol98], R. -P. Holzapfel introduced two rational invariants of a two-dimensional complex orbifold (X, B) (in the sense of [Hol98]), called the Euler height $\mathbf{e}(X, B)$ (see [Hol98], 3. 3.) and the Signature height $\mathbf{sign}(X, B)$ ([Hol98], 3. 4.), which in the case of a smooth surface are the usual Euler number and the signature. In the general case, Euler- and Signature height contain contributions coming from the orbital cycle B, a marked cycle of X, which should be thought as a virtual branch locus of a finite covering of X. Most important result on these invariants is the nice property that they behave multiplicatively under finite coverings with respect to the degree. In particular, if $Y \xrightarrow{f} (X, B)$ is a uniformization of (X, B), i. e. a smooth surface which is a finite Galois cover of (X, B), ramified exactly over B, then $c_2(Y) = deg(f)\mathbf{e}(X, B)$, $\mathrm{sign}(Y) = deg(f)\mathbf{sign}(X, B)$. In our case, $X_{\Gamma'}$ is an uniformization of the orbifold $(X_\Gamma, Q_1, Q_2, Q_3)$. Since $X_{\Gamma'}$ is a fake projective plane, we have $e(X_{\Gamma'}) = 3$, $\mathrm{sign}(X_{\Gamma'}) = 1$. Applying Holzapfels formulas [Hol98] prop. 3.3.4, and prop. 3.4.3, we get $e(X_\Gamma) = 3$, $\mathrm{sign}(X_\Gamma) = 1$. The birational resolution map ρ consists of 9 monoidal transformations. Then, using [Hol98], p. 142 ff, we obtain $e(\widetilde{X_\Gamma}) = 3+9$, $sign(\widetilde{X_\Gamma}) = 1-9$. The other invariants are immediately obtained using facts from the general theory mentioned at the end of section 2.2. □

Proof of Proposition 4.1 continued. From the proof of the above Proposition we can deduce that there are no more branch points than we have found. Namely, if we assume that there are more, and knowing that no branch curves exist, we immediately obtain a contradiction to the equality between the orbital invariants $c_2(X_{\Gamma'}) = 7\mathbf{e}(X_\Gamma) = 7(e(X_\Gamma) - \sum(1 - 1/d_i))$ (by definition we have $\mathbf{e}(X_\Gamma) = e(X_\Gamma) - \sum(1 - 1/d_i)$, where sum is taken over the branch locus, and d_i appears in the type (d_i, e_i) of the branch point Q_i, see [Hol98], 3. 3). Let us give an argument that no branch curves are possible. Such a curve must be subball quotient $C = \mathbb{D}/G$, with $\mathbb{D} \subset \mathbb{B}$, $\mathbb{D} \cong \mathbb{B}_1$ a disc fixed by a reflection in Γ and $G \subset \Gamma$ an arithmetic subgroup consisting of all elements in Γ acting on $\mathbb{D}$. Then G is commensurable to a group of elements with reduced norm 1 in an order of a quaternion subalgebra $Q \subset D$, which is necessarily a division algebra. But for dimension reasons D cannot contain quaternion algebras. Therefore C doesn't exist. □

In the next step we compute the irregularity and the geometric genus.

Proposition 4.3. $q(\widetilde{X_\Gamma}) = p_g(\widetilde{X_\Gamma}) = 0$.

Proof. Due to the fact that $\chi(\widetilde{X_\Gamma}) = 1 - q(\widetilde{X_\Gamma}) + p_g(\widetilde{X_\Gamma}) = 1$, by preceding propostion 4.2, it suffices to show that one of the above invariants vanishes, let's say $p_g(\widetilde{X_\Gamma}) = \dim H^0(\widetilde{X_\Gamma}, \Omega^2_{\widetilde{X_\Gamma}})$. We know that $p_g(X_{\Gamma'}) = 0$. Let $\Omega^2_{X_\Gamma}$ denote the space of holomorphic 2-forms on (the singular surface) X_Γ. Then $\Omega^2_{X_\Gamma}$ is exactly the space of $\langle\zeta\rangle$-invariant 2-forms on $X_{\Gamma'}$, i. e. $\Omega^2_{X_\Gamma} = (\Omega^2_{X_{\Gamma'}})^{\langle\zeta\rangle}$ (see [Gri76]). On the other hand we have an isomorphism between $\Omega^2_{\widetilde{X_\Gamma}}$ and $\Omega^2_{X_\Gamma}$ (again by [Gri76]). Altogether, $p_g(\widetilde{X_\Gamma}) = 0$. □

Let us remark at this stage, that even if we know some invariants of $\widetilde{X_\Gamma}$, we still need to determine the Kodaira dimension in order to classify $\widetilde{X_\Gamma}$, since there exist surfaces with these invariants in every Kodaira dimension. We will determine $\mathrm{kod}(\widetilde{X_\Gamma})$ discussing the second plurigenus of $\widetilde{X_\Gamma}$. Using an argument of Ishida [Ish88] we first prove

Lemma 4.4. *Let $A_2(\Gamma, j)$ denote the space of Γ-automorphic forms of weight 2 with respect to the Jacobian determinant as the factor of automorphy and let $P_2(\widetilde{X_\Gamma})$ be the second plurigenus of $\widetilde{X_\Gamma}$. Then $P_2(\widetilde{X_\Gamma}) = \dim A_2(\Gamma, j)$.*

Proof. We can identify $A_2(\Gamma, j)$ with the space of $\langle\zeta\rangle$-invariant sections $H^0(X_{\Gamma'}, \mathcal{K}_{X_{\Gamma'}}^{\otimes 2})^{\langle\zeta\rangle}$. Every such section can be regarded as a holomorphic section $s \in H^0(X_\Gamma^{sm}, \mathcal{K}_{X_\Gamma^{sm}}^{\otimes 2})$, where $X_\Gamma^{sm} = X_\Gamma \backslash \{Q_1, Q_2, Q_3\}$ denotes the smooth part of X_Γ. We can think of X_Γ^{sm} as an open dense subset of $\widetilde{X_\Gamma}$. The crucial point is to show that s has a holomorphic continuation along the exceptional locus. For this, let (s) be the divisor of $\widetilde{X_\Gamma}$ corresponding to s and write (s) in three different ways as $(s) = a_{i,1}E_{i,1} + a_{i,2}E_{i,2} + a_{i,3}E_{i,3} + D_i$, $i = 1, 2, 3$, with $E_{i,j}$ as in Proposition 4.1 and no $E_{i,j}$ is contained in the support of D_i. Then, we have to show that $a_{i,j}$ are nonnegative integers. Let K denote the canonical divisor of $\widetilde{X_\Gamma}$. We notice that (s) and $2K$ are linearly equivalent. With our convention stated in Proposition 4.1 the adjunction formula gives the following intersection numbers:

$$\begin{aligned} ((s) \cdot E_{i,1}) &= (2K \cdot E_{i,1}) = 2, \\ ((s) \cdot E_{i,2}) &= (2K \cdot E_{i,2}) = 0, \\ ((s) \cdot E_{i,3}) &= (2K \cdot E_{i,3}) = 0. \end{aligned} \tag{4.1}$$

On the other hand,

$$\begin{aligned} ((s) \cdot E_{i,1}) &= (a_{i,1}E_{i,1} + a_{i,2}E_{i,2} + a_{i,3}E_{i,3} + D_i \cdot E_{i,1}) \\ &= -3a_{i,1} + a_{i,2} + d_{i,1}, \\ ((s) \cdot E_{i,2}) &= a_{i,1} - 2a_{i,2} + a_{i,3} + d_{i,2}, \\ ((s) \cdot E_{i,3}) &= a_{i,2} - 2a_{i,3} + d_{i,3}, \end{aligned} \tag{4.2}$$

with some nonnegative integers $d_{i,j}$. Now, (4.1) and (4.2) lead to a system of linear equations, which has positive solutions $a_{i,j}$, $j = 1, 2, 3$. □

In [Hir66], F. Hirzebruch developed a formula for the dimension of spaces of automorphic forms $A_k(\Delta, j)$ of weight k with respect to a discrete and cocompact group which acts properly discontinously on some bounded hermitian symmetric domain with emphasis on ball quotient case. Let us recall this formula in the case of quotients of the n-dimensional ball:

Let Δ be a discrete group which acts properly discontinuously on the n-dimensional ball $\mathbb{B}_n$ with a compact fundamental domain. For $\delta \in \Delta$ let Δ_δ be the centralizer of δ in Δ, $Fix(\delta)$ the fixed point set of δ in $\mathbb{B}_n$, and $m(\delta)$

the number of elements in Δ_δ which act trivially on $Fix(\delta)$. If $r(\delta)$ denotes the dimension of $Fix(\delta)$ let $R(r(\delta),k)$ be the coefficient of $z^{r(\delta)}$ in the formal power series expansion of $(1-z)^{k(n+1)-1}\prod_{i=r(\delta)+1}^{n}\frac{1}{1-\nu_i+\nu_i z}$, where $\nu_{r(\delta)+1},\ldots,\nu_n$ are the eigenvalues of δ normal to $Fix(\delta)$. $R(r(\delta),k)$ is a polynomial in k of degree $r(\delta)$. Hirzebruch's result is:

$$\dim A_k(\Delta,j)=\sum_{[\delta]}\frac{e(\Delta_\delta\backslash Fix(\delta))j_\delta^k}{m(\delta)(r(\delta)+1)}R(r(\delta),k), \tag{4.3}$$

where $e(\Delta_\delta\backslash Fix(\delta))$ is the "virtual Euler number" (in the sense of [Hir66]), j_δ is the Jacobian determinant evaluated at an arbitrary point of $Fix(\delta)$ and the sum is running over all conjugacy classes $[\delta]$ of elements with fixed points in $\mathbb{B}_n$.
We apply this formula to the group Γ, which after some elementary calculations in combination with Lemma 4.4 gives the following result.

Proposition 4.5. $P_2(\widetilde{X_\Gamma})=1$.

We use the above Proposition and an argument of Keum (see [Keu08]) to get

Corollary 4.6. $\mathrm{kod}(\widetilde{X_\Gamma})=1$. *Moreover, $\widetilde{X_\Gamma}$ is a minimal elliptic surface.*

Proof. If $\widetilde{X_\Gamma}$ were of general type, the Riemann-Roch Theorem would imply $P_2(\widetilde{X_\Gamma})\geq 2$, which contradicts the Proposition 4.5. Also $\widetilde{X_\Gamma}$ is not rational by Castelnuovo's criterion. Assuming $\mathrm{kod}(\widetilde{X_\Gamma})=0$, $\widetilde{X_\Gamma}$ can only an Enriques surface because of its topological invariants and because the selfintersection number of the canonical divisor is zero by Proposition 4.2 $\widetilde{X_\Gamma}$ is not a blow-up of an Enriques surface. The canonical divisor K_{X_Γ} of the normal surface X_Γ is a $\mathbb{Q}$-Cartier divisor such that $K_{X_{\Gamma'}}$ is numerically equivalent to $\psi^*K_{X_\Gamma}$, where $\psi: X_{\Gamma'}\longrightarrow X_\Gamma$ denotes the degree-7 quotient morphism. Working with intersection numbers of $\mathbb{Q}$-divisors, it follows that $(K_{X_{\Gamma'}}\cdot K_{X_{\Gamma'}})=deg(\psi)(K_{X_\Gamma}\cdot K_{X_\Gamma})$ and therefore $(K_{X_\Gamma}\cdot K_{X_\Gamma})=9/7$. This implies, with $\rho: K_{\widetilde{X_\Gamma}}\longrightarrow K_{X_\Gamma}$ being the minimal desingularization, that $(\rho^*K_{X_\Gamma}\cdot K_{\widetilde{X_\Gamma}})=(K_{X_\Gamma}\cdot K_{X_\Gamma})>0$. Therefore $K_{\widetilde{X_\Gamma}}$ is not numerically equivalent to zero. But the canonical divisor of an Enriques surface is numerically trivial. Contradiction. Since $c_2(\widetilde{X_\Gamma})=12$ and $c_1^2(\widetilde{X_\Gamma})=0$, $\widetilde{X_\Gamma}$ has to be minimal by the classification theory (see [BHPVdV04]). □

Remark 4.7. In the above mentioned recent paper [Keu08], J. H. Keum studies systematically quotients of fake projective planes by finite groups of automorphisms. According to his results the minimal desingularizations of such quotients can only be surfaces of general type or surfaces of Kodaira dimension 1.

5 Another elliptic surface

In this section we will study the ball quotient by an arithmetic group which contains Γ. Its desingularization turns out to be another elliptic surface, which has been already studied by Ishida [Ish88] p-adically. From there we obtain the elliptic fibration on both of these surfaces.

5.1 Passage to the normalizer

In general, the normalizer $N\Lambda$ in $\mathbf{G}(\mathbb{R})$ of a principal arithmetic group $\Lambda \subset \mathbf{G}(\mathbb{Q})$ is a maximal arithmetic group ([BP89], prop. 1. 4.). In fact, for the principal group $\Gamma = \Gamma_{\mathcal{O},b}$, we infer from [PY07], 5. 4. that the normalizer $\tilde{\Gamma}$ of Γ in the projective group $\mathbb{P}\mathbf{G}(\mathbb{R}) = \mathbf{G}(\mathbb{R})/\{\text{center}\}$ contains Γ with index 3. Morover, $\tilde{\Gamma} \cap \mathbf{G}_b(\mathbb{Q}) = \Gamma$. It is easily shown, that the matrix $\tau = \left(\begin{smallmatrix} 0 & 0 & \alpha \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{smallmatrix}\right)$ has the order three, normalizes Γ, and lastly represents a class in $\mathbb{P}\mathbf{G}_b(\mathbb{R}) \cong \mathrm{PU}(H_b)$. Consequently, $X_{\tilde{\Gamma}} = X_\Gamma/\langle\tau\rangle$. Let $X_\Gamma \xrightarrow{\varphi} X_{\tilde{\Gamma}}$ denote the canonical projection. In the same way as in the Lemma 4.1, we obtain the following

Lemma 5.1. *The ball quotient $X_{\tilde{\Gamma}}$ is smooth outside four points Q, P_1, P_2, P_3, which are cyclic quotient singularities of type $(7,3)$ (represented by Q) and $(3,2)$ (represented by P_1, P_2, P_3). The minimal resolution of Q is a Hirzebruch-Jung string $A_1 + A_2 + A_3$ of type $(-3)(-2)(-2)$ and each of P_i-s is resolved by a Hirzebruch-Jung string $F_{i,1} + F_{i,2}$ of type (-2) (-2), $i = 1, 2, 3$.*

Proof. Let $g \in D$ be the element introduced at the begining of section 4. Using the relation $\tau g = g^\sigma \tau$, which in fact holds for any $g \in D$, it is directly checked that τ permutes the three lines x, x^σ and $x^{\sigma\sigma}$ which are fixed by Z. Consequently the three singular points Q_1, Q_2, Q_3 of X_Γ are mapped to one single point $Q \in X_{\tilde{\Gamma}}$ by φ. This point remains a quotient singularity of type $(7,3)$. There is at least one singularity more, call it P_1, coming from the positive definite eigenline of τ corresponding to the eigenvalue $\omega = \frac{1}{2}(-1+\sqrt{-3})$. It is a quotient singularity of type $(3,2)$ since around it τ acts as $diag(\omega, \omega^2)$. In order to show that there are two more singularities, we make use of the relation between orbifold invariants of X_Γ and $X_{\tilde{\Gamma}}$. We know namely that $\mathbf{e}(X_\Gamma) = 3\mathbf{e}(X_{\tilde{\Gamma}})$. Furthermore, the (topological) Euler number $e(X_{\tilde{\Gamma}})$ equals 3. In the same way as in the proof of Proposition 4.1 we exclude branch curves. Then by definition $\mathbf{e}(X_{\tilde{\Gamma}}) = 3 - 6/7 - \sum_{k=1}^{r}(1 - 1/d_k)$, where r denotes the number of elliptic branch points $\neq Q$, and d_k appears in the type (d_k, e_k) of the k-th branch point. On the other hand $\mathbf{e}(X_\Gamma) = 3/7 = 3\mathbf{e}(X_{\tilde{\Gamma}})$. This holds only if $r = 3$ and $d_k = 3$ for all k, as a short calculation shows. This gives two further branch points P_2 and P_3. Using the same argument with the signature height we conclude that all branch points, not of type $(7,3)$ must be of type $(3,2)$. Namely, assuming the opposite we always get a contradiction to the equation $\mathbf{sign}(X_\Gamma) = 3\mathbf{sign}(X_{\tilde{\Gamma}})$. □

Again, we can ask about the structure of the minimal desingularization $\widetilde{X_{\tilde{\Gamma}}}$ of

$X_{\tilde{\Gamma}}$ as we did before for X_Γ. With the same methods used in the investigation of X_Γ we get

Proposition 5.2. *$\widetilde{X_{\tilde{\Gamma}}}$ is a minimal elliptic surface of Kodaira dimension one with $p_g = q = 0$.*

Proof. The topological invariants are computed using the Euler- and Signature height presented in the proof of Proposition 4.2 and Lemma 5.1. We get the same topological invariants as in Proposition 4.2: $e(\widetilde{X_{\tilde{\Gamma}}}) = 12$, $\tau(\widetilde{X_{\tilde{\Gamma}}}) = -8$. The assertion about the irregularity and the geometric genus follows directly from the (proof of) Proposition 4.3, since we have $\chi(\widetilde{X_{\tilde{\Gamma}}}) = 1$ again. Lastly, we can apply Hirzebruch's formula in order to compute the second plurigenus, since the proof of Lemma 4.4 works in the present case without any change. Therefore, we can identify the second plurigenus with the dimension $\dim A_2(\tilde{\Gamma}, j)$ of the corresponding space of automorphic forms. By elementary calculations, (4.3) leads to $P_2(\widetilde{X_{\tilde{\Gamma}}}) = 1$. As in the proof of Corollary 4.6 we deduce the asserted Kodaira dimension. □

5.2 Elliptic fibration

We have to mention, that alternatively to the approach we have described, for the proof of Proposition 5.2 we can completely refer to [Ish88], some of whose arguments we have already used before. There, the author a priori works over a non-archimedian field, but most of his arguments work independently of it. Morover, in [Ish88], section 4, the singular fibers of the elliptic fibration on $X_{\tilde{\Gamma}}$ are completely determined. The non-multiple singular fibers are closely related to the exceptional curves on $\widetilde{X_{\tilde{\Gamma}}}$.To be precise, we have

Theorem 5.3 (compare [Ish88], section 4). *$\widetilde{X_{\tilde{\Gamma}}}$ admits an elliptic fibration f over $\mathbb{P}_1$. f has exactly one multiple fiber of multiplicity 2 and one multiple fiber of multiplicity 3. Furthermore, it has four non-multiple singular fibers, all of type I_3 (in Kodaira's notation) $B_0 = A_2 + A_3 + D_0$, $B_1 = F_{1,1} + F_{1,2} + D_1$, $B_2 = F_{2,1} + F_{2,2} + D_2$, $B_3 = F_{3,1} + F_{3,2} + D_3$.*

We can now use the knowledge of the elliptic fibration on $X_{\tilde{\Gamma}}$ to reconstruct the elliptic fibration on X_Γ. Since we know the finite covering φ, this is not a difficulty anymore. Again the non-multiple singular fibers contain the exceptional curves. For the proof of the next Theorem we can also refer to [Keu06] whose starting point was exactly the determination of the elliptic fibration.

Theorem 5.4 (see [Keu06], Proposition 2. 1.). *The elliptic fibration g on X_Γ over $\mathbb{P}_1$ has exactly two multiple fibers, one of multiplicity two and one of multiplicity three. It has four non-multiple singular fibers, one of type I_9: $C_0 = E_{1,2} + E_{1,3} + E_{2,2} + E_{2,3} + E_{3,2} + E_{3,3} + D_{1,0} + D_{2,0} + D_{3,0}$, and three of type I_1: $A_i = D_i^{'}$, $i = 1, 2, 3$. There $D_i^{'}$ is the inverse image of D_i under φ.*

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Interface and mixed boundary value problems on n-dimensional polyhedral domains

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Abstract. Let $\mu \in \mathbb{Z}_+$ be arbitrary. We prove a well-posedness result for mixed boundary value/interface problems of second-order, positive, strongly elliptic operators in weighted Sobolev spaces $\mathcal{K}^\mu_a(\Omega)$ on a bounded, curvilinear polyhedral domain Ω in a manifold M of dimension n. The typical weight η that we consider is the (smoothed) distance to the set of singular boundary points of $\partial\Omega$. Our model problem is $Pu := -\operatorname{div}(A\nabla u) = f$, in Ω, $u = 0$ on $\partial_D\Omega$, and $D^P_\nu u = 0$ on $\partial_\nu\Omega$, where the function $A \geq \epsilon > 0$ is piece-wise smooth on the polyhedral decomposition $\bar\Omega = \cup_j \bar\Omega_j$, and $\partial\Omega = \partial_D\Omega \cup \partial_N\Omega$ is a decomposition of the boundary into polyhedral subsets corresponding, respectively, to Dirichlet and Neumann boundary conditions. If there are no interfaces and no adjacent faces with Neumann boundary conditions, our main result gives an isomorphism $P : \mathcal{K}^{\mu+1}_{a+1}(\Omega) \cap \{u = 0 \text{ on } \partial_D\Omega,\ D^P_\nu u = 0 \text{ on } \partial_N\Omega\} \to \mathcal{K}^{\mu-1}_{a-1}(\Omega)$ for $\mu \geq 0$ and $|a| < \eta$, for some $\eta > 0$ that depends on Ω and P but not on μ. If interfaces are present, then we only obtain regularity on each subdomain Ω_j. Unlike in the case of the usual Sobolev spaces, μ can be arbitrarily large, which is useful in certain applications. An important step in our proof is a *regularity* result, which holds for general strongly elliptic operators that are not necessarily positive. The regularity result is based, in turn, on a study of the geometry of our polyhedral domain when endowed with the metric $(dx/\eta)^2$, where η is the weight (the smoothed distance to the singular set). The well-posedness result applies to positive operators, provided the interfaces are smooth and there are no adjacent faces with Neumann boundary conditions.

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Introduction

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded set. Consider the boundary value problem

$$\begin{cases} \Delta u = f & \text{in } \Omega \\ u|_{\partial\Omega} = g, & \text{on } \Omega, \end{cases} \tag{1}$$

where Δ is the Laplace operator. For Ω smooth, this boundary value problem has a unique solution $u \in H^{s+2}(\Omega)$ depending continuously on $f \in H^s(\Omega)$ and $g \in H^{s+3/2}(\partial\Omega)$, $s \geq 0$. See the books of Evans [25], Lions and Magenes [49], or Taylor [72] for proofs of this basic and well known result.

It is also well known that this result does not extend to non-smooth domains Ω. For instance, Jerison and Kenig prove in [35] that if $g = 0$ and $\Omega \subset \mathbb{R}^n$, $n \geq 3$, is an open, bounded set such that $\partial\Omega$ is Lipschitz, then Equation (1) has a unique solution in $W^{s,p}(\Omega)$ depending continuously on $f \in W^{s-2,p}(\Omega)$ if, and only if, $(1/p, s)$ belongs to a certain explicit hexagon. They also prove a similar result if $\Omega \subset \mathbb{R}^2$. A consequence of this result is that the smoothness of the solution u (measured by the order s of the Sobolev space $W^{s,p}(\Omega)$ containing it) will not exceed, in general, a certain bound that depends on the domain Ω and p, even if f is smooth.

In addition to the Jerison and Kenig paper mentioned above, a deep analysis of the difficulties that arise for $\partial\Omega$ Lipschitz is contained in the papers of Babuška [4], Baouendi and Sjöstrand [9], Băcuţă, Bramble, and Xu [14], Babuška and Guo [31, 30], Brown and Ott [13], Jerison and Kenig [33, 34], Kenig [38], Kenig and Toro [39], Koskela, Koskela and Zhong [43, 44], Mitrea and Taylor [58, 60, 61], Verchota [73], and others (see the references in the aforementioned papers). Results more specific to curvilinear polyhedral domains are contained in the papers of Costabel [17], Dauge [19], Elschner [20, 21], Kondratiev [41, 42], Mazya and Rossmann [54], Rossmann [63] and others. Excellent references are also the monographs of Grisvard [27, 28] as well as the recent books [45, 46, 52, 53, 62], where more references can be found.

In this paper, we consider the boundary value problem (1) when Ω is a *bounded curvilinear polyhedral domain* in $\mathbb{R}^n$, or, more generally, in a manifold M of dimension n and, Poisson's equation $\Delta u = f$ is replaced by a positive, strongly elliptic scalar equation. We define curvilinear polyhedral domains inductively in Section 2. We allow polyhedral domains to be disconnected for technical reasons, more precisely, for the purpose of defining them inductively. Our results, however, are formulated for connected polyhedral domains. Many polyhedral

domains are Lipschitz domains, but not all. This fact is discussed in detail by Vogel and Verchota in [74], where they also prove that the harmonic measure is absolutely continuous with respect to the Lebesgue measure on the boundary as well as the solvability of Equation (1) if $f = 0$ and $g \in L^{2-\epsilon}(\partial\Omega)$, thus generalizing several earlier, classical results. See also the excellent book [50]. The generalized polyhedra we considered are of combinatorial type if no cracks are present. (For a discussion of more general domains, see the references [68, 74, 75].)
Instead of working with the usual Sobolev spaces, as in several of the papers mentioned above, we shall work in some weighted analogues of these papers. Let $\Omega^{(n-2)} \subset \partial\Omega$ be the set of singular (or non-smooth) boundary points of Ω, that is, the set of points $p \in \partial\Omega$ such $\partial\Omega$ is not smooth in a neighborhood of p. We shall denote by $\eta_{n-2}(x)$ the distance from a point $x \in \Omega$ to the set $\Omega^{(n-2)}$. We agree to take $\eta_{n-2} = 1$ if there are no such points, that is, if $\partial\Omega$ is smooth. We then consider the weighted Sobolev spaces

$$\mathcal{K}_a^{\mu}(\Omega) = \{u \in L^2_{\text{loc}}(\Omega),\, \eta_{n-2}^{|\alpha|-a}\partial^{\alpha}u \in L^2(\Omega), \text{ for all } |\alpha| \le \mu\}, \quad \mu \in \mathbb{Z}_+, \quad (2)$$

which we endow with the induced Hilbert space norm. A similar definition yields the weighted Sobolev spaces $\mathcal{K}_a^{s}(\partial\Omega)$, $s \in \mathbb{R}_+$. By including an extra weight h in the above spaces we obtain the spaces $h\mathcal{K}_a^{\mu}(\Omega)$ and $h\mathcal{K}_a^{s}(\partial\Omega)$ (where h is required to be an admissible weight, see Definition 3.8 and Subsection 5.1). These spaces are closely related to the weighted Sobolev spaces on non-compact manifolds considered, for example in the references [41, 42, 46, 54, 62, 63] mentioned above, as well as in the works of Erkip and Schrohe [22], Grubb [29], Schrohe [65], as well as the sequence of papers of Schrohe and Schulze [66, 67] concerning related results on boundary value problems on non-compact manifolds and, more generally, on the analysis on non-compact manifolds.
The main result of this article, Theorem 1.2 applies to operators with *piecewise smooth coefficients*, such as $\operatorname{div} a\nabla u = f$, where a is allowed to have only jumps across the interface. A simplified version of that result, when formulated for the Laplace operator Δ on $\mathbb{R}^n$ with Dirichlet boundary conditions, reads as follows. In this theorem and throughout this paper, Ω will always denote an open set.

Theorem 0.1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded, curvilinear polyhedral domain and $\mu \in \mathbb{Z}_+$. Then there exists $\eta > 0$ such that the boundary value problem* (1) *has a unique solution $u \in \mathcal{K}_{a+1}^{\mu+1}(\Omega)$ for any $f \in \mathcal{K}_{a-1}^{\mu-1}(\Omega)$, any $g \in \mathcal{K}_{a+1/2}^{\mu+1/2}(\partial\Omega)$, and any $|a| < \eta$. This solution depends continuously on f and g. If $a = \mu = 0$, this solution is the solution of the associated variational problem.*

The case $n = 2$ of the above theorem is Theorem 6.6.1 in the excellent monograph [45]. Results in higher dimensions related to the ones in our paper can be found, for instance, in [19, 45, 51, 54, 62]. These works also use the framework of the $\mathcal{K}_a^{\mu}(\Omega)$ spaces. The spaces $h\mathcal{K}_a^{\mu}(\Omega)$, with h an admissible weight are somewhat more general (see Definition 3.8 for a definition of admissible weights). We also take the dimension n of the ambient Euclidean space $\mathbb{R}^n \supset \Omega$ to be arbitrary. Furthermore, we impose mixed Dirichlet/Neumann boundary conditions and allow the boundary conditions to change along $(n-2)$-dimensional, piecewise smooth hypersurfaces in each hyperface of Ω. To handle this situation, we include in the singular set of Ω all points where the boundary conditions change, giving rise to a polyhedral structure on Ω which is not entirely determined by geometry, but also takes into account the specifics of the boundary value problem. However, we consider only second order, strongly elliptic systems. For $n = 3$, mixed boundary value problems for such systems in polyhedral domains were studied in weighted L^p spaces by Mazya and Rossmann [54] using point estimates for the Green's function [55]. Since we work in L^2-based spaces, we use instead coercive estimates, which directly generalize to arbitrary dimension and to transmission problems. We use manifolds in order to be able to prove estimates inductively. The method of layer potentials seems to give more precise results, but is less elementary (see for example [38, 59, 60, 75]). Solvability of mixed boundary value problems from the point of view of parametrices and pseudodifferential calculus can be found in the papers by Eskin [23, 24], Vishik and Eskin [76, 77, 78], and Boutet de Monvel [10, 11] among others.

As we have already pointed out, it is not possible to obtain full regularity in the usual Sobolev spaces, when the smoothness of the solution as measured by $\mu + 1$ in Theorem 0.1 is too large. On the other hand, the weighted Sobolev spaces have proved themselves to be as convenient as the usual Sobolev spaces in applications. Possible applications are to partial differential equations, algebraic geometry, representation theory, and other areas of pure and applied mathematics, as well as to other areas of science, such as continuum mechanics, quantum mechanics, and financial mathematics. See for example [7, 8, 48], where optimal rates of convergence were obtained for the Finite element method on 3D polyhedral domains and for 2D transmission problems using weighted Sobolev spaces.

The paper is organized as follows. In Section 1, we introduce the mixed boundary value/interface problem that we study, namely Equation (6), and state the main results of the paper, Theorem 1.1 on the regularity of (6) in weighted spaces of arbitrarily high Sobolev index, and Theorem 1.2 on the solvability of (6) under additional conditions on the operator (positivity) and on the domain (smooth interfaces and no two adjacent faces with Neumann boundary conditions). In Section 2, we give a notion of curvilinear, polyhedral domain in arbitrary dimension using induction, then we specialize to the familiar case of polygonal domains in $\mathbb{R}^2$ and polyhedral domains in $\mathbb{R}^3$, and describe the desingularization $\Sigma(\Omega)$ of the domain Ω in these familiar settings. Before discussing the desingularization in higher dimension, we recall briefly needed notions from the theory of Lie manifolds with boundary in Section 3. Then, in Section 4 we show that $\Sigma(\Omega)$, also defined by induction on the dimension, naturally carries a structure of Lie manifold with boundary. We also discuss the construction of the canonical weight function r_Ω, which extends smoothly to $\Sigma(\Omega)$ and is comparable to the distance to the singular set. In turn, the Lie manifold structure on $\Sigma(\Omega)$ allows to identify the spaces $\mathcal{K}^{\mu}_{a}(\Omega)$, $\mu \in \mathbb{Z}_+$, with standard Sobolev spaces on $\Sigma(\Omega)$, and hence lead to a definition of the weighted Sobolev spaces on the boundary $\mathcal{K}^{s}_{a}(\partial\Omega)$, $s \in \mathbb{R}$. Lastly Section 6 contains the proofs of the main results and most of lemmas of the paper; in particular, it contains a proof of the weighted Hardy-Poincaré inequality used to establish positivity or strict coercivity for the problem of Equation (6). An earlier version of this paper was first circulated as an IMA Preprint in August 2004.

We conclude this Introduction with a word on notation. By Ω we always mean an open set in $\mathbb{R}^n$. By a diffeomorphisms, we mean a C^∞ invertible map with C^∞ inverse. By C we shall denote a generic constant that may change from line to line. We also denote $\mathbb{Z}_+ = \{0, 1, 2, 3, \ldots\}$.

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1 The problem and statement of the main results

We begin by introducing the class of differential operators and the associated mixed Dirichlet-Neumann boundary value/interface problem that will be the object of study. For simplicity, we consider primarily the scalar case, although our results extend to systems as well. Then, we state the main results of this article, namely the regularity and the well-posedness of the mixed boundary value/interface problem (6) in weighted Sobolev spaces for n-dimensional, curvilinear polyhedral domains $\Omega \subset \mathbb{R}^n$. These are stated in Theorems 1.2 and 1.1.

Our analysis is general enough to extend to a bounded subdomain $\Omega \subset M$ of a compact Riemannian manifold M. Initially the reader may assume the polyhedron is straight, that is, informally, that every j-dimensional component of the boundary, $j = 1, \ldots, n-1$ is a subset of an affine space. A complete definition of a curvilinear polyhedral domain is given in Section 2.

1.1 The differential operator P and the associated problem

Let us denote by $\Omega \subset \mathbb{R}^n$ a bounded, curvilinear stratified polyhedral domain (see Definition 2.1). The domain Ω need not be connected, nor convex. We assume that we are given a decomposition

$$\overline{\Omega} = \cup_{j=1}^{N} \overline{\Omega}_j, \tag{3}$$

where Ω_j are disjoint polyhedral subdomains. In particular, every face of Ω is also a face of one of the domains Ω_j. This is possible since the faces of Ω are not determined only by the geometry of Ω. As discussed in Section 4, a face of codimension 1 of Ω is called a hyperface. For well-posedness results, we shall assume that

$$\Gamma = \cup_{j=1}^{N} \partial\Omega_j \setminus \partial\Omega, \tag{4}$$

is a finite collection of disjoint, smooth $(n-1)$-hypersurfaces. We observe that, since each Ω_j is a polyhedron, each component of Γ intersects $\partial\Omega$ transversely. We refer to Γ as the *interface*.

We also assume that the boundary of Ω is partition into two *disjoint* subsets

$$\partial\Omega = \partial_D\Omega \cup \partial_N\Omega, \tag{5}$$

with $\partial_N\Omega$ consisting of a union of open faces of Ω. For well-posedness results, we shall assume that $\partial_N\Omega$ does not contain adjacent faces of $\partial\Omega$.

We are interested in studying the following mixed boundary value/interface problem for a certain class of elliptic, scalar operators P described below:

$$\begin{cases} Pu = f & \text{on } \Omega, \\ u|_{\partial_D\Omega} = g_D & \text{on } \partial_D\Omega, \\ D^P_\nu u|_{\partial_N\Omega} = g_N & \text{on } \partial_N\Omega, \\ u^+ = u^-, \ D^{P+}_\nu u = D^{P-}_\nu u & \text{on } \Gamma. \end{cases} \tag{6}$$

Above, ν is the unit outer normal to $\partial\Omega$, which is defined almost everywhere, D^P_ν is the conormal derivative associated to the operator P (see (10)), and $\pm$ refers to one-sided, non-tangential limits at the interface Γ. We observe that $D^{P\pm}_\nu$ is well-defined a.e. on each side of the interface Γ, since each smooth component of Γ is the boundary of exactly two adjacent polyhedral domains Ω_j, by (4). The coefficients of P will have in general jump discontinuities along Γ.

We next introduce the class of differential operators that we consider. At first, the reader may assume $P = -\Delta$, the Laplace operator. We shall write $Re(z) := \frac{1}{2}(z + \overline{z})$, or simply $Re\, z$ for the real part of a complex number z.

Let $u \in H^2_{\text{loc}}(\Omega)$. We shall study the following scalar, differential operator in divergence form

$$Pu(x) = -\sum_{j,k=1}^{n} \partial_j \big[A_{jk}(x)\partial_k u(x)\big] + \sum_{j=1}^{n} B_j(x)\partial_j u(x) + C(x)u(x). \tag{7}$$

The coefficients A_{jk}, B_j, C are real valued with only jump discontinuities on the interface Γ, the operator P is required to be uniformly strongly elliptic and to satisfy another positivity condition. More precisely, the coefficients of P are assumed to satisfy:

$$A_{jk},\, B_j,\, C \in \oplus_{j=1}^{N} \mathcal{C}^\infty(\overline{\Omega_j}) \cap L^\infty(\overline{\Omega}) \tag{8a}$$

$$Re\Big(\sum_{j,k=1}^{n} [A_{jk}(x)]\xi_j\overline{\xi}_k\Big) \geq \epsilon \sum_{j=1}^{n} |\xi_j|^2, \quad \forall \xi_j \in \mathbb{C},\ \forall x \in \Omega, \quad \text{and} \tag{8b}$$

$$2C(x) - \sum_{j=1}^{n} \partial_j B_j(x) \geq 0, \tag{8c}$$

for some $\epsilon > 0$.

For scalar equations, one may weaken the uniform strong ellipticity condition (8b), but this is not needed for our purposes. Our results extend to systems satisfying the *strong Legendre–Hadamard* condition, namely

$$Re\Big(\sum_{j,k=1}^{n} \sum_{p,q=1}^{m} [A_{jk}(x)]_{pq}\xi_{jp}\overline{\xi}_{kq}\Big) \geq \epsilon \sum_{j=1}^{n}\sum_{p=1}^{m} |\xi_{jp}|^2, \quad \forall \xi_{jp} \in \mathbb{C}, \tag{9}$$

and a condition on the lower-order terms equivalent to (8c). This condition is not satisfied however by the system of anisotropic elasticity in $\mathbb{R}^3$, for which nevertheless the well-posedness result holds if the elasticity tensor is positive definite on symmetric matrices [56].

In (8a), the "regularity condition on the coefficients of P" means that the coefficients and their derivatives of all orders have well-defined limits from each side of Γ, but as equivalence classes in L^∞ they may have jump discontinuities along the interface. This condition can be relaxed, but it allows us to state a regularity result of arbitrary order in each subdomains for the solution to the problem (6). The conormal derivative associated to the operator P is formally defined by:

$$D_P^\nu u(x) = \sum_{i,j=1}^{n} \nu_i\, A_{ij}\partial_j u(x), \tag{10}$$

where $\nu = (\nu^i)$ is the unit outer normal vector to the boundary of Ω. We give meaning to (10) in the sense of trace at the boundary. In particular, for u regular enough $D_\nu^P u$ is defined almost everywhere on the boundary as a non-tangential limit.

The problem (6) with $g_D = 0$ is interpreted in a weak (or variational) sense, using the bilinear form $B(u, v)$ defined by:

$$B(u, v) := \sum_{j,k=1}^{n} \big(A_{jk}\partial_k u, \partial_j v\big) + \sum_{j=1}^{n} \big(B_j\partial_j u, v\big) + \big(Cu, v\big), \tag{11}$$

which is well-defined for any $u, v \in H^1(\Omega)$. Then, (6) is weakly equivalent to

$$B(u, v) = (f, v)_{L^2(\Omega)} + (g_N, v)_{\partial_N\Omega}, \tag{12}$$

where the second parenthesis denotes the pairing between a distribution and a (suitable) function. The jump or *transmission* conditions, $u^+ = u^-$, $D^P_\nu u^+ = D^P_\nu u^-$ at the interface Γ follow from the weak formulation and the H^1-regularity of weak solutions, and hence justify passing from the strong formulation (6) to the weak one (12). Otherwise, in general, the difference $D^{P+}_\nu u - D^{P-}_\nu u$ may be non-zero and may be included as a distributional term in f.

Condition (8c) implies the Hardy-Poincaré type inequality

$$ReB(u,u) > C(\eta_{n-2}u, \eta_{n-2}u)_{L^2}, \tag{13}$$

if there are no adjacent faces with Neumann boundary conditions and the interface is smooth. In fact, it is enough to assume that the latter is satisfied instead of (8c). For applications, however, it is more convenient to have the concrete condition (8c).

Problems of the form (6) arise in many applications. An important example is given by (linear) elastostatics. In this case, $[Pu]^i = -\sum_{jkl=1}^3 \partial_j\, C^{ijkl}\, \partial_k u^l$, $i = 1, 2, 3$, where C is the fourth-order elasticity tensor, modelling the response of an elastic body under small deformations. Dirichlet or displacement boundary conditions correspond to clamping (parts of) the boundary, while Neumann or traction boundary conditions correspond to loading mechanically (parts of) the boundary. Interfaces arise due to the use of different materials. A careful analysis of mixed Dirichlet/Neumann boundary value problems for linear elastostatics in 3-dimensional curvilinear, polyhedral domains, was carried out by two of the authors in [56]. There, the concept of a "domain with polyhedral structure" is more general than in this paper and includes cracks. In [48], they studied mixed boundary value/interface problems and the implementation of the Finite Element Method on "domains with polygonal structure" with non-smooth interfaces (see also [15]). The results of this paper can be extended to include domains with cracks, as in [56] and [48], but the topological machinery used there, including the notion of an "unfolded boundary" [19] in arbitrary dimensions is significantly more complex. (See [12] for related results.)

1.1.1 Operators on manifolds

We turn to consider the assumptions on P when the domain Ω is a curvilinear, polyhedral domain in a manifold M of the same dimension. Let then E be a vector bundle on M endowed with a hermitian metric. A coordinate free expression of the conditions in Equations (8a)–(8c) is obtained as follows. We assume that there exist a metric preserving connection $\nabla : \Gamma(E) \to \Gamma(E \otimes T^*M)$, a smooth endomorphism $A \in \mathrm{End}(E \otimes T^*M)$, and a first order differential operator $P_2 : \Gamma(E) \to \Gamma(E)$ with smooth coefficients such that

$$A + A^* \geq 2\epsilon I \text{ for some } \epsilon > 0. \tag{14}$$

Then we define $P_1 = \nabla^* A \nabla$ and $P = P_1 + P_2$. In particular, the operator P will satisfy the strong Lagrange–Hadamard condition in a neighborhood of Ω in M.

Note that if $\Omega \subset \mathbb{R}^n$ and the vector bundle E is trivial, then the condition of (14) reduces to the conditions of (8), by taking ∇ to be the trivial connection. We can allow A to have jump discontinuities as well along polyhedral interfaces.

1.2 The main results

We are ready to state the principal results of this paper. *We continue to assume hypotheses* (3)–(5) *on the domain* Ω *and its decomposition into disjoint subdomains* Ω_j *separated by the interface* Γ.
We begin with a regularity results for solutions to the problem (6) in weighted Sobolev spaces $h\mathcal{K}^\mu_a$, $\mu \in \mathbb{Z}_+$, $a \in \mathbb{R}$, where

$$\mathcal{K}^\mu_a(\Omega) := \{u \in L^2_{\text{loc}}(\Omega),\, \eta_{n-2}^{|\alpha|-a}\partial^\alpha u \in L^2(\Omega), \text{ for all } |\alpha| \leq \mu\}, \quad \mu \in \mathbb{Z}_+,$$

and

$$h\mathcal{K}^\mu_a(\Omega) := \{hu,\, u \in \mathcal{K}^\mu_a(\Omega)\}.$$

(See Section 5 for a detailed discussion and main properties of these spaces.) Above, η_{n-2} is the distance to the singular set in Ω given in Definition 2.5, while h is a so-called admissible weight described in Definition 3.8. Initially, the reader may assume that $h = r_\Omega^b$, $b \in \mathbb{R}$, where r_Ω is a function comparable to the distance function η_{n-2} close to the singular set, but with better regularity than η_{n-2} away from the singular set. (We refer again to Subsection 5.1 for more details). The weight h is important in the applications of the theory developed here for numerical methods, where appropriate choices of h yield quasi-optimal rates of convergence for the Finite Element approximation to the weak solution of the problem (6) (see [6, 7, 8, 48]).

Theorem 1.1. *Let* $\Omega \subset \mathbb{R}^n$ *be a bounded, curvilinear polyhedral domain of dimension* n. *Assume that the operator* P *satisfies conditions* (8a) *and* (8b). *Let* $\mu \in \mathbb{Z}_+$, $a \in \mathbb{R}$, *and* $u \in h\mathcal{K}^1_{a+1}(\Omega)$ *be such that* $Pu \in h\mathcal{K}^{\mu-1}_{a-1}(\Omega_j)$, *for all* j, $u|_{\partial_D\Omega} \in h\mathcal{K}^{\mu+1/2}_{a+1/2}(\partial_D\Omega)$, $D^P_\nu u|_{\partial_N\Omega} \in h\mathcal{K}^{\mu-1/2}_{a-1/2}(\partial_N\Omega)$. *If* h *is an admissible weight, then* $u \in h\mathcal{K}^{\mu+1}_{a+1}(\Omega_j)$, *for all* $j = 1, \ldots, N$, *and*

$$\|u\|_{h\mathcal{K}^{\mu+1}_{a+1}(\Omega_j)} \leq C\Big(\sum_{k=1}^N \|Pu\|_{h\mathcal{K}^{\mu-1}_{a-1}(\Omega_k)} + \|u\|_{h\mathcal{K}^0_{a+1}(\Omega)} + \|u|_{\partial_D\Omega}\|_{h\mathcal{K}^{\mu+1/2}_{a+1/2}(\partial_D\Omega)} + \|u|_{\partial_N\Omega}\|_{h\mathcal{K}^{\mu-1/2}_{a-1/2}(\partial_N\Omega)}\Big) \tag{15}$$

for a constant $C = C(\Omega, P, \mu, a, h) > 0$, *independent of* u.

The proof of the regularity theorem exploits Lie manifolds and their structure to reduce to the classical case of bounded, smooth domains. The proof can be found in Section 6. Note that in this theorem we do not require the interfaces to be smooth and we allow for adjacent faces with Neumann boundary conditions. Under additional conditions on the set Ω and its boundary ensuring strict coercivity of the bilinear form B of equation (11), we obtain a well-posedness result for problem (6). In [48], two of the authors obtained a well-posedness result in an augmented space on polygonal domains with "Neumann-Neumann vertices," *i.e.,* vertices for which both sides joining at the vertex are given Neumann boundary conditions, and for which the interface Γ is not smooth. Such result is based on specific spectral properties of operator pencils near the vertices and is not easily extendable to higher dimension. Note that $\mathcal{K}^\mu_a(\Omega) = h\mathcal{K}^\mu_0(\Omega)$ for a suitable admissible weight h and hence there is no loss of generality to assume $a = 0$ in Theorem 1.1. We will use the same reasoning to simplify the statements of the following results.

Theorem 1.2. *Let $\Omega \subset \mathbb{R}^n$ be a bounded, connected curvilinear polyhedral domain of dimension n. Assume that $\partial\Omega_N$ does not contain any two adjacent hyperfaces, that $\partial_D\Omega$ is not empty, and that the interface Γ is smooth. In addition, assume that the operator P satisfies conditions* (8). *Let $\mathcal{W}_\mu(\Omega)$, $\mu \in \mathbb{Z}_+$, be the set of admissible weights h such that the map $\tilde{P}(u) := (Pu, u|_{\partial_D\Omega}, D^P_\nu u|_{\partial_N\Omega})$ establishes an isomorphism*

$$\tilde{P} : \{u \in \bigoplus_{j=1}^{N} h\mathcal{K}^{\mu+1}_1(\Omega_j) \cap h\mathcal{K}^1_1(\Omega),\ D^P_\nu u^+ = D^P_\nu u^- \ \text{on}\ \Gamma\}$$
$$\to \bigoplus_{j=1}^{N} h\mathcal{K}^{\mu-1}_{-1}(\Omega_j) \oplus h\mathcal{K}^{\mu+1/2}_{1/2}(\partial_D\Omega) \oplus h\mathcal{K}^{\mu-1/2}_{-1/2}(\partial_N\Omega).$$

Then the set $\mathcal{W}_\mu(\Omega)$ is an open set containing 1.

Theorem 1.2 reduces to a well-known, classical result when Ω is a smooth bounded domain. (See Remark 6.11 for a result on smooth domains that is not classical.) The same is true for the following result, Theorem 1.3, which works for general domains on manifolds. Note however that for manifolds it is more difficult to express the coercive property, so for more complete results we restrict to the case of operators of Laplace type.

Theorem 1.3. *Let $\Omega \subset M$ be a bounded, connected curvilinear polyhedral domain of dimension n. Assume that every connected component of Ω has a non-empty boundary and that the operator P satisfies condition* (14). *Assume additionally that no two adjacent hyperfaces of $\partial\Omega$ are endowed with Neumann boundary conditions and that the interface Γ is smooth. Let $c \in \mathbb{C}$ and $\mathcal{W}'_\mu(\Omega)$ be the set of admissible weights h such that the map $\tilde{P}_c(u) := (Pu + cu, u|_{\partial\Omega}, D^P_\nu u|_{\partial\Omega})$ establishes an isomorphism*

$$\tilde{P}_c : \{u \in \bigoplus_{j=1}^{N} h\mathcal{K}^{\mu+1}_1(\Omega_j) \cap h\mathcal{K}^1_1(\Omega),\ u^+ = u^-,\ D^P_\nu u^+ = D^P_\nu u^- \ \text{on}\ \Gamma\}$$
$$\to \bigoplus_{j=1}^{N} h\mathcal{K}^{\mu-1}_{-1}(\Omega_j) \oplus h\mathcal{K}^{\mu+1/2}_{1/2}(\partial_D\Omega) \oplus h\mathcal{K}^{\mu-1/2}_{-1/2}(\partial_N\Omega).$$

Then the set $\mathcal{W}'_\mu(\Omega)$ *is an open set, which contains* 1 *if the real part of* c *is large or if* $P = \nabla^* A \nabla$ *with* A *satisfying* (14).

For the rest of this section, Ω and P will be as in Theorem 1.2. We discuss some immediate consequences of Theorem 1.2. Analogous results can be obtained from Theorem 1.3, but we will not state them explicitly. The continuity of the inverse of $\tilde{P}$ is made explicit in the following corollary.

Corollary 1.4. *Let* A *satisfy* (14). *There exists a constant* $C = C(\Omega, P, \mu, a, h) > 0$, *independent of* f, g_D, *and* g_N, *such that*

$$\|u\|_{h\mathcal{K}^1_1(\Omega)} + \|u\|_{h\mathcal{K}^{\mu+1}_1(\Omega_j)} \leq C\big(\sum_{j=1}^{N} \|Pu\|_{h\mathcal{K}^{\mu-1}_{-1}(\Omega_j)} + \|u|_{\partial_D\Omega}\|_{h\mathcal{K}^{\mu+1/2}_{1/2}(\partial_D\Omega)} + \|D^P_\nu u|_{\partial_N\Omega}\|_{h\mathcal{K}^{\mu+1/2}_{1/2}(\partial_N\Omega)}\big),$$

for any $u \in h\mathcal{K}^1_1(\Omega)$ *and any* j.

From the fact that η_{n-2} is equivalent to r_Ω by Proposition 4.9 and Corollary 4.11, we obtain the following corollary.

Corollary 1.5. *Let* A *satisfy* (14). *There exists* $\eta > 0$ *such that*

$$(P, D^P_\nu) : \{u \in \bigoplus_{j=1}^{N} \mathcal{K}^{\mu+1}_{a+1}(\Omega_j) \cap \mathcal{K}^1_{a+1}(\Omega),\ u|_{\partial_D\Omega} = 0, D^P_\nu u^+ = D^P_\nu u^- \text{ on } \Gamma\} \to \bigoplus_{j=1}^{N} \mathcal{K}^{\mu-1}_{a-1}(\Omega_j) \oplus \mathcal{K}^{\mu-1/2}_{a-1/2}(\partial_N\Omega)$$

is an isomorphism for all $\mu \in \mathbb{Z}_+$ *and all* $|a| < \eta$.

Note above and in what follows that the interface matching condition $u^+ = u^-$ follows from $u \in \mathcal{K}^1_{a+1}(\Omega)$.

Proof. From the results in Sections 5 and 5.1, $\mathcal{K}^{\mu+1}_{a+1} = r^a_\Omega \mathcal{K}^{\mu+1}_1$ and r^a_Ω is an admissible weight for any $a \in \mathbb{R}$. The result then follows from the fact that $\mathcal{W}_\mu(\Omega)$ is an open set containing the weight 1 by Theorem 1.2. ☐

The following corollary gives a characterization of the set $\mathcal{W}_\mu(\Omega)$ in the spirit of [15]. There, similar arguments give that for $n = 2$ the constant η in the previous corollary is $\eta = \pi/\alpha_M$, where α_M is the largest angle of Ω. See also [42].

Corollary 1.6. *Let* $h = r^a_\Omega$ *and* A *satisfy* (14). *Assume that for all* $\lambda \in [0, 1]$ *the map*

$$(P, D^P_\nu) : \{u \in h^\lambda \mathcal{K}^1_1(\Omega),\ u|_{\partial_D\Omega} = 0, \quad D^P_\nu u|_{\partial_N\Omega} = 0\} \to h^\lambda \mathcal{K}^{-1}_{-1}(\Omega)$$

is Fredholm. Then $h \in \mathcal{W}_\mu(\Omega)$.

The corollary holds for more general weights $h = \prod_H x_H^{a_H}$, where x_H is the distance to an hyperface H at infinity (see Section 5.1), as long as all $a_H \geq 0$ or all $a_H \leq 0$.

Proof. We proceed as in [15]. The family $P_\lambda := h^{-\lambda} P h^\lambda$ is continuous for $\lambda \in [0,1]$, consists of Fredholm operators by hypothesis, and is invertible for $\lambda = 0$ by Theorem 1.2. It follows that the family P_λ consists of Fredholm operators of index zero. To prove that these operators are isomorphisms, it is hence enough to prove that they are either injective or surjective. Assume first that $a \geq 0$ in the definition of h. Then $\mathcal{K}_1^{1+\lambda}(\Omega) = h^\lambda \mathcal{K}_1^1(\Omega) \subset \mathcal{K}_1^1(\Omega)$. Therefore P is injective on

$$h^\lambda \mathcal{K}_1^1(\Omega) \cap \{u|_{\partial_D \Omega} = 0,\ D_P^\nu u|_{\partial_N \Omega} = 0\}.$$

This, in turn, gives that P_λ is injective.
Assume that $a \leq 0$ and consider

$$P_\lambda : h^\lambda \mathcal{K}_1^1(\Omega) \cap \{u|_{\partial\Omega} = 0,\ D_P^\nu u|_{\partial_N \Omega} = 0\} \to h^\lambda \mathcal{K}_{-1}^{-1}(\Omega). \tag{16}$$

We have $(P_\lambda)^* = (P^*)_{-\lambda}$. The same argument as above shows that P_λ^* is injective, and hence that it is an isomorphism, for all $0 \leq \lambda \leq 1$. Hence P_λ is an isomorphism for all $0 \leq \lambda \leq 1$. ☐

2 Polyhedral domains

In this section we introduce the class of domains to which the results of the previous sections apply. We then specialize to domains in 2 and 3 dimensions and provide ample examples. The reader may at first concentrate on this case. We describe how to desingularize the domain in arbitrary dimension later in the paper, using the theory of Lie manifolds, which we recall in the next section.
Let Ω be a proper open set in $\mathbb{R}^n$ or more generally in a smooth manifold M of dimension n. Our main focus is the analysis of partial differential equations on Ω, specifically the mixed boundary value/interface problem (6). For this reason, we give Ω a structure that is not entirely determined by geometry, rather it takes into account the boundary and interface conditions for the operator P in problem (6).
We assume that Ω is given together with a smooth stratification:

$$\Omega^{(0)} \subset \Omega^{(1)} \subset \ldots \subset \Omega^{(n-2)} \subset \Omega^{(n-1)} := \partial\Omega \subset \Omega^{(n)} := \bar{\Omega}. \tag{17}$$

We recall that a *smooth stratification* $S_0 \subset S_1 \subset \ldots \subset X$ of a topological space X is an increasing sequence of closed sets $S_j = S_j(X)$ such that each point of X has a neighborhood that meets only finitely many of the sets S_j, S_0 is a discrete subset, $S_{j+1} \smallsetminus S_j$, $j \geq 0$, is a disjoint union of smooth manifolds of dimension $j+1$, and $X = \cup S_j$. Some of the sets S_j may be empty for $0 \leq j \leq j_0 < \dim(X)$.

We will always assume that the stratification $\{\Omega^{(j)}\}$ *satisfies the condition that* $\Omega^{(j)} \smallsetminus \Omega^{(j-1)}$ *has finitely many connected components, for all* j. This assumption is automatically satisfied if Ω is bounded, and it is not crucial, but simplifies some of the later constructions.

We proceed by induction on the dimension to define a polyhedral structure on Ω. Our definition is very closely related to that of Whitney stratified spaces [79]. We first agree that a curvilinear polyhedral domain of dimension $n = 0$ is simply a finite set of points. Then, we assume that we have defined curvilinear polyhedral domains in dimension $\leq n-1$, $n \geq 1$, and define a curvilinear polyhedral domain in a manifold M of dimension n next. We shall denote by B^l the open unit ball in $\mathbb{R}^l$ and by $S^{l-1} := \partial B^l$ its boundary. In particular, we identify $B^0 = \{1\}$, $B^1 = (-1, 1)$, and $S^0 = \{-1, 1\}$.

Definition 2.1. Let M be a smooth manifold of dimension $n \geq 1$. Let $\Omega \subset M$ be an open subset endowed with the stratification (17). Then $\Omega \subset M$ is a *stratified, curvilinear polyhedral domain* if for every point $p \in \partial\Omega$, there exist a neighborhood V_p in M such that:

(i) if $p \in \Omega^{(l)} \setminus \Omega^{(l-1)}$, $l = 1, \ldots, n-1$, there is a curvilinear polyhedral domain $\omega_p \subset S^{n-l-1}$, $\overline{\omega_p} \neq S^{n-l-1}$, and

(ii) a diffeomorphism $\phi_p : V_p \to B^{n-l} \times B^l$ such that $\phi_p(p) = 0$ and

$$\phi_p(\Omega \cap V_p) = \{rx', \, 0 < r < 1, \, x' \in \omega_p\} \times B^l, \tag{18}$$

inducing a homeomorphism of stratified spaces.

Given any $p \in \partial\Omega$, let $0 \leq \ell(p) \leq n-1$ be the smallest integer such that $p \in \Omega^{(\ell(p))}$, but $p \notin \Omega^{(\ell(p)-1)}$ (by convention we set $\Omega^{(l)} = \emptyset$ if $l < 0$). By construction, $\ell(p)$ is unique given p. Then, the domain $\omega_p \subset S^{n-\ell(p)-1}$ in the definition above will be called the *link of* Ω *at* p. We identify the "ball" $B^0 = \{1\}$ and the "sphere" $S^0 = \partial B^1 = \{-1, 1\}$. In particular if $\ell(p) = n-1$, then ω_p is a point.

The notion of a stratified polyhedron is well known in the literature (see for example the monograph [71]). However, our definition is more general, and well suited for applications to partial differential equations. See the papers of Babuška and Guo [5], Mazya and Rossmann [54], and Verchota and Vogel [74, 75] for related definitions. We remark that, according to the above definition, Ω does not need to be bounded, nor connected, nor convex. *For applications to the analysis of boundary value/interface problems, however, we will always assume* Ω *is connected.* The boundary $\partial\Omega$ need not be connected either, but it does have finitely many connected components. We also stress that polyhedral domains will always be open subsets.

The condition $\overline{\omega_p} \neq S^{n-l-1}$ can be relaxed to $\omega_p \neq S^{n-l-1}$, thus allowing for cracks and slits, but not punctured domains of the form $M \smallsetminus \{p\}$. We will not pursue this generality in the paper, given also that submanifolds of codimension greater than 2 consists of irregular boundary points for elliptic equations and may lead to ill-posedness in boundary value problems. We refer to the articles [48, 56] for a detailed analysis of polyhedral domains with cracks in 2 and 3 dimensions.

We continue with some comments on Definition 2.1 before providing several concrete examples in dimension $n = 1, 2, 3$. We denote by tB^l the ball of radius t in $\mathbb{R}^l$, $l \in \mathbb{N}$, centered at the origin. We also let tB^0 to be a point independent of t. Sometimes it is convenient to replace Condition (18) with the equivalent condition that there exist $t > 0$ such that

$$\phi_p(\Omega \cap V_p) = \{rx',\, 0 < r < t, x' \in \omega_p\} \times tB^l. \tag{19}$$

We shall interchange conditions (18) and (19) at will from now on. For a cone or an infinite wedge, $t = +\infty$, so cones and wedges are particular examples of polyhedral domain.

We have the following simple result that is an immediate consequence of the definitions.

Proposition 2.2. *Let $\psi : M \to M'$ be a diffeomorphism and let $\Omega \subset M$ be a curvilinear polyhedral domain. Then $\psi(\Omega)$ is also a curvilinear polyhedral domain.*

Next, we introduce the *singular set* of Ω, $\Omega_{\text{sing}} := \Omega^{(n-2)}$. A point $p \in \Omega^{(n-2)}$ will be called a *singular point* for Ω. We recall that a point $x \in \partial\Omega$ is called a *smooth boundary point* of Ω if the intersection of $\partial\Omega$ with a small neighborhood of p is a smooth manifold of dimension $n-1$. In view of Definition 2.1, the point p is smooth if ϕ_p satisfies

$$\phi_p(\Omega \cap V_p) = (0, t) \times B^{n-1}. \tag{20}$$

This observation is consistent with ω_p being a point in this case, since it is a polyhedral domain of dimension 0.

Any point $p \in \partial\Omega$ that is not a smooth boundary point in this sense is a singular point. But the singular set may include other points as well, in particular the points where the boundary conditions change, *i.e.,* the points of the boundary of $\partial_D\Omega$ in $\partial\Omega$, and the points where the interface Γ meets $\partial\Omega$. It is known [36, 37] that the solution to the problem (6) near such points behaves in a similar way as in the neighborhood of non-smooth boundary points. We call the non-smooth points in $\partial\Omega$ the *true* or *geometric* singular points, while we call all the other singular points *artificial* singular points.

The true singular points can be characterized by the condition that the domain ω_p of Definition 2.1 be an "irreducible" subset of the sphere S^{n-l-1}, in the sense of the following definition.

Definition 2.3. A subset $\omega \subset S^{n-1} := \partial B^n$, the unit sphere in $\mathbb{R}^n$ will be called *irreducible* if $\mathbb{R}_+\omega := \{rx',\, r > 0, x' \in \omega\}$ cannot be written as $V + V'$ for a linear subspace $V \subset \mathbb{R}^k$ of dimension ≥ 1 and V' an arbitrary subset of $\mathbb{R}^{n-k}$. (The sum does not have to be a direct sum and, in fact, V' is not assumed to be an affine subspace.)

For example, $(0,\alpha) \subset S^1$ is irreducible if, and only if, $\alpha \neq \pi$. A subset $\omega \subset S^{n-1}$ strictly contained in an open half-space is irreducible, but the intersection of S^{n-1}, $n \geq 2$, with an open half-space is not irreducible.
If $p \in \Omega^{(0)}$, then we shall call p a *vertex* of Ω and we shall interpret the condition (18) as saying that ϕ_p defines a diffeomorphism such that

$$\phi_p(\Omega \cap V_p) = \{rx',\, 0 < r < t, x' \in \omega_p\}. \tag{21}$$

This interpretation is consistent with our convention that the set B^0 (the zero dimensional unit ball) consists of a single point. We shall call any open, connected component of $\Omega^{(1)} \smallsetminus \Omega^{(0)}$ an (open) *edge* of Ω, necessarily a smooth curve in M. Similarly, any open, connected component of $\Omega^{(j)} \smallsetminus \Omega^{(j-1)}$ shall be called a (open) *j–face* if $2 \leq j \leq n-1$. A $n-1$-face will be called a *hyperface.* A j–face H is a smooth manifold of dimension j, but in general it is not a curvilinear polyhedral domain (except if $n = 2$), because there might not exist a j-manifold containing the closure of H in $\partial\Omega$. This point will be addressed in terms of the desingularization $\Sigma(\Omega)$ of Ω constructed in Section 4.

Notations 2.4. *From now on, Ω will denote a curvilinear polyhedral domain in a manifold M of dimension n with given stratification $\Omega^{(0)} \subset \Omega^{(1)} \subset \ldots \subset \Omega^{(n)} := \overline{\Omega}$.*

Some or all of the sets $\Omega^{(j)}$, $j = 0, \ldots, n-2$, in the stratification of Ω may be empty. In fact, $\Omega^{(n-2)}$ is empty if, and only if, $\overline{\Omega}$ is a smooth manifold, possibly with boundary, a particular case of a curvilinear, stratified polyhedron. Finally we introduce the notion of distance to the singular set $\Omega^{(n-2)}$ of Ω (if not empty) on which the constructions of the Sobolev spaces $\mathcal{K}^\mu_a(\Omega)$ given in Section 5 is based. If $\Omega^{(n-2)} = \emptyset$, we let $\eta_{n-2} \equiv 1$.

Definition 2.5. Let Ω be a curvilinear, stratified polyhedral domain of dimension n. The distance function $\eta_{n-2}(x)$ from x to the singular set $\Omega^{(n-2)}$ is

$$\eta_{n-2}(x) := \inf_\gamma \ell(\gamma), \tag{22}$$

where $\ell(\gamma)$ is the length of the curve γ, and γ ranges through all smooth curves $\gamma : [0,1] \to \overline{\Omega}$, $\gamma(0) = x$, $p := \gamma(1) \in \Omega^{(n-2)}$.

If Ω is not bounded, for example Ω is an infinite cone, then we modify the definition of the distance function as follows:

$$\eta_{n-2}(x) := \chi(\inf_\gamma \ell(\gamma)), \qquad \text{where}$$
$$\chi \in C^\infty([0,+\infty)), \quad \chi(s) = \begin{cases} s, & 0 \leq s \leq 1 \\ \geq 1, & s \geq 1 \\ 2, & s \geq 3, \end{cases} \tag{23}$$

which has the effect of making η_{n-2} a bounded function.

2.1 Curvilinear polyhedral domains in 1, 2, and 3 dimensions

In this subsection we give some examples of curvilinear polyhedral domains Ω in $\mathbb{R}^2$, in S^2, or in $\mathbb{R}^3$. These examples are crucial in understanding Definition 2.1, which we specialize here for $n = 2$, $n = 3$. The desingularization $\Sigma(\Omega)$ and the function r_Ω will be introduced in the next subsection in these special cases. We have already defined a polyhedron in dimension 0 as a finite collection of points. Accordingly, a subset $\Omega \subset \mathbb{R}$ or $\Omega \subset S^1$ is a *curvilinear polyhedral domain* if, and only if, it is a finite union of open intervals.
Let M be a smooth 2-manifold or $\mathbb{R}^2$. Definition 2.1 can be more explicitly stated as follows.

Definition 2.6. A subset $\Omega \subset M$ together with smooth stratification $\Omega^{(0)} \subset \Omega^{(1)} \equiv \partial\Omega \subset \Omega^{(2)} \equiv \Omega$ will be called *a curvilinear, stratified polygonal domain* if, for every point of the boundary $p \in \partial\Omega$, there exists a neighborhood $V_p \subset M$ of p and a diffeomorphism $\phi_p : V_p \to B^2$, $\phi_p(p) = 0$, such that:

(a) $\phi_p(V_p \cap \Omega) = \{\, (r\cos\theta, r\sin\theta),\ 0 < r < 1,\ \theta \in \omega_p \,\}$, where ω_p is a union of open intervals of the unit circle such that $\overline{\omega_p} \neq S^1$;

(b) if $p \in \Omega^{(1)} \smallsetminus \Omega^{(0)}$, then ω_p is exactly an interval of length π.

Any point $p \in \Omega^{(0)}$ is a *vertex* of Ω, and p is a true vertex precisely when ω_p is not an interval of length π. The open, connected components of $\partial\Omega \smallsetminus \Omega^{(0)}$ are the (open) *sides* of Ω. In view of condition (b) above, sides are smooth curves $\gamma_j : [0,1] \to M$, $j = 1, \ldots, N$, with no common interior points. Recall that by hypothesis, there are finitely many vertices and sides. The condition that $\overline{\omega_p} \neq S^1$ implies that either a side γ_j has a vertex in common with another side γ_k or γ_j is a closed smooth curve or an unbounded smooth curve. In the special case $\Omega^{(1)} \smallsetminus \Omega^{(0)} = \emptyset$, Ω has only isolated conical points (see Example 2.11 in the next subsection), while if $\Omega^{(0)} = \emptyset$, Ω has smooth boundary.

Notations 2.7. *Any curvilinear, stratified polygon in $\mathbb{R}^2$ will be denoted by $\mathbb{P}$ and its stratification by $\mathbb{P}^{(0)} \subset \mathbb{P}^{(1)} = \partial\mathbb{P} \subset \mathbb{P}^{(2)} = \overline{\mathbb{P}}$.*

Let now M be a smooth 3-manifold or $\mathbb{R}^3$. Definition 2.1 can also be stated more explicitly.

Definition 2.8. A subset $\Omega \subset M$ together with a smooth stratification $\Omega^{(0)} \subset \Omega^{(1)} \subset \Omega^{(2)} \equiv \partial\Omega \subset \Omega^{(3)} \equiv \overline{\Omega}$ will be called *a curvilinear, stratified polyhedral domain* if, for every point of the boundary $p \in \partial\Omega$, there exists a neighborhood $V_p \subset M$ of p and a diffeomorphism $\phi_p : V_p \to B^l \times B^{3-l}$, $\phi_p(p) = 0$, such that:

(a) $\phi_p(V_p \cap \Omega) = \{\, (y, rx'),\ y \in B^l,\ 0 < r < t,\ x' \in \omega_p \,\}$, where $t \in (0, +\infty]$ and $\omega_p \subset S^{2-l}$ is such that $\overline{\omega_p} \neq S^{2-l}$;

(b) if $l = 0$ (*i.e.,* if $p \in \Omega^{(0)}$), then $\omega_p \subset S^2$ is a stratified, curvilinear polygonal domain;

(c) if $l = 1$ (*i.e.*, if $p \in \Omega^{(1)} \smallsetminus \Omega^{(0)}$), then ω_p is a finite, disjoint union of finitely many open intervals in S^1 of total length less than 2π.

(d) if $l = 2$ then p is a smooth boundary point;

(e) ϕ_p preserves the stratifications.

Each point $p \in \Omega^{(0)}$ is a *vertex* of Ω and p is a true vertex precisely when ω_p is an irreducible subset of S^2 (according to Definition 2.3). The open, connected components of $\Omega^{(1)} \smallsetminus \Omega^{(0)}$ are the *edges* of Ω, smooth curves with no interior common points by condition (c) above. The open, connected components of $\Omega^{(2)} \smallsetminus \Omega^{(1)}$, smooth surfaces with no common interior points, are the *faces* of Ω. Recall that by hypothesis, there are only finitely many vertices, edges, and faces in Ω. The condition that $\overline{\omega_p}$ be not the whole sphere S^{2-l} ($l = 1, 0$) implies that either an edge γ_j has a vertex in common with another edge γ_k or γ_j is a closed smooth curve or an unbounded smooth curve (such as in a wedge), and similarly for faces. Again, in the the case $\Omega^{(1)} = \Omega^{(0)}$, Ω has only isolated conical points, in the case $\Omega^{(0)} = \emptyset$, Ω has only edge singularities, and in the case $\Omega^{(1)} = \Omega^{(0)} = \emptyset$, Ω is smooth.
The following subsection contains several examples.

2.2 Definition of $\Sigma(\Omega)$ and of r_Ω if $n = 2$ or $n = 3$

We now introduce the desingularization $\Sigma(\Omega)$ for some of the typical examples of curvilinear polyhedral domains in $n = 2$ or $n = 3$. The desingularization of a domain $\Omega \subset M$ depends in general on M, but we do not explicitly show this dependence in the notation, and generally ignore it in order to streamline the presentation, given that the manifold M will be mostly implicit. Associated to the singularization is the function r_Ω, which is comparable with the distance to the singular set η_{n-2} but is more regular. We also frame these definitions as examples. The general case (of which the examples considered here are particular cases) is in Section 4. The reader can skip this part at first reading. The case $n = 2$ of a polygonal domain $\mathbb{P}$ in $\mathbb{R}^2$ is particularly simple. We use the notation in Definition 2.6.

Example 2.9. The desingularization $\Sigma(\mathbb{P})$ of $\mathbb{P}$ will replace each of the vertices A_j, $j = 1, \dots, k$, of $\mathbb{P}$ with a segment of length $\alpha_j > 0$, where α_j is the magnitude of the angle at A_j (if A_j is an artificial vertex, then $\alpha_j = \pi$). We can realize $\Sigma(\mathbb{P})$ in three dimensions as follows. Let θ_j be the angle in a polar coordinates system (r_j, θ_j) centered at A_j. Let ϕ_j be a smooth function on $\mathbb{P}$ that is equal to 1 on $\{r_j < \epsilon\}$ and vanishes outside $V_j := \{r_j < 2\epsilon\}$. By choosing $\epsilon > 0$ small enough, we can arrange that the sets V_j do not intersect. We define then

$$\Phi : \overline{\mathbb{P}} \smallsetminus \{A_1, A_2, \dots, A_k\} \to \mathbb{P} \times \mathbb{R} \subset \mathbb{R}^3$$

by $\Phi(p) = (p, \sum \phi_j(p)\theta_j(p))$. Then $\Sigma(\mathbb{P})$ is (up to a diffeomorphism) the closure in $\mathbb{R}^3$ of $\Phi(\mathbb{P})$. The desingularization map is $\kappa(p, z) = p$. The structural Lie algebra of vector fields $\mathcal{V}(\mathbb{P})$ on $\Sigma(\mathbb{P})$ is given by (the lifts of) the smooth vector fields X on $\overline{\mathbb{P}} \smallsetminus \{A_1, A_2, \ldots, A_k\}$ that on $V_j = \{r_j < 2\epsilon\}$ can be written as

$$X = a_r(r_j, \theta_j) r_j \partial_{r_j} + a_\theta(r_j, \theta_j)\partial_{\theta_j}, \tag{24}$$

with a_r and a_θ smooth functions of (r_j, θ_j) on $[0, 2\epsilon) \times [0, \alpha_j]$. We can take $r_\Omega(x) := \psi(x) \prod_{j=1}^k r_j(x)$, where ψ is a smooth, nowhere vanishing function on $\Sigma(\Omega)$. (Such a factor ψ can always be introduced, and the function r_Ω is determined only up to this factor. We shall omit this factor in the examples below.)

The examples of a domain with a single edge or of a domain with a single vertex are among of the most instructive.

Example 2.10. Let first Ω be the wedge

$$\mathbb{W} := \{(r\cos\theta, r\sin\theta, z),\ 0 < r, 0 < \theta < \alpha, z \in \mathbb{R}\}, \tag{25}$$

where $0 < \alpha < 2\pi$, and $x = r\cos\theta$ and $y = r\sin\theta$ define the usual cylindrical coordinates (r, θ, z), with $(r, \theta, z) \in [0, \infty) \times [0, 2\pi) \times \mathbb{R}$. Then the manifold of generalized cylindrical coordinates is, in this case, just the domain of the cylindrical coordinates on $\overline{\mathbb{W}}$:

$$\Sigma(\mathbb{W}) = [0, \infty) \times [0, \alpha] \times \mathbb{R}.$$

The desingularization map is $\kappa(r, \theta, z) = (r\cos\theta, r\sin\theta, z)$ and the structural Lie algebra of vector fields of $\Sigma(\mathbb{W})$ is

$$a_r(r, \theta, z) r\partial_r + a_\theta(r, \theta, z)\partial_\theta + a_z(r, \theta, z) r\partial_z,$$

where a_r, a_z, and a_θ are smooth functions on $\Sigma(\mathbb{W})$. Note that the vector fields in $\mathcal{V}(\mathbb{W})$ may not extend to the closure $\overline{\mathbb{W}}$. We can take $r_\Omega = r$, the distance to the Oz-axis.

At this stage, we can describe a domain with one conical point and its desingularization in any dimension.

Example 2.11. Let next Ω be *a domain with one conical point*, that is, Ω is a curvilinear, stratified polyhedron in $\mathbb{R}^n$ such that $\Omega^{(j)} = \Omega^{(0)}$ for all $1 \leq j \leq n-2$. We assume Ω is bounded for simplicity. Let $p \in \Omega^{(0)}$ denote the single vertex of Ω. There exists a neighborhood V_p of p such that, up to a local change of coordinates,

$$V_p \cap \Omega = \{rx',\ 0 \leq r < \epsilon, x' \in \omega\}, \tag{26}$$

for some smooth, connected domain $\omega \subset S^{n-1} := \partial B^n$. Then we can realize $\Sigma(\Omega)$ in $\mathbb{R}^{2n}$ as follows. Assume $p = 0$, the origin, for simplicity. We define $\Phi(x) = (x, |x|^{-1}x)$ for $x \neq p$, where $|x|$ is the distance from x to the origin (*i.e.,* to p). The set $\Sigma(\Omega)$ is defined to be the closure of the range of Φ. The map κ is the projection onto the first n components. The map κ is one-to-one, except that $\kappa^{-1}(p) = \{p\} \times \omega$. We can take $r_\Omega(x) = |x|$. The Lie algebra of vector fields $\mathcal{V}(\Omega)$ consists of the vector fields on $\Sigma(\Omega)$ that are tangent to $\kappa^{-1}(p)$. This example is due to Melrose [57].

Example 2.12. Let $\Omega \subset \mathbb{R}^3$ be a convex polyhedral domain, such that all edges are straight segments. To construct $\Sigma(\Omega)$, we combine the ideas used in the previous examples. First, for each edge e we define (r_e, θ_e, z_e) to be a coordinate system aligned to that edge and such that $\theta_e \in (0, \alpha_e)$, as in Example 2.10. Let $v_1, v_2, \dots, v_b$ be the set of vertices of Ω and $e_1, \dots, e_a$ be the set of edges. Then, for x not on any edge of Ω, we define $\Phi(x) \in \mathbb{R}^{3+a+b}$ by

$$\Phi(x) = \big(x, \theta_{e_1}, \theta_{e_2}, \dots, \theta_{e_a}, |x - v_1|^{-1}(x - v_1), \dots, |x - v_b|^{-1}(x - v_b)\big)\,.$$

The desingularization $\Sigma(\Omega) \subset \mathbb{R}^{3+a+b}$ is defined as the closure of the range of Φ. The resulting set will be a manifold with corners with several different types of hyperfaces. Namely, the manifold $\Sigma(\Omega)$ will have a hyperface for each face of Ω, a hyperface for each edge of Ω, and, finally, a hyperface for each vertex of Ω. The last two types of hyperfaces are the so-called *hyperfaces at infinity* of $\Sigma(\Omega)$. Let x_H be the distance to the hyperface H. We can take then $r_\Omega = \prod_H x_H$, where H ranges through the hyperfaces at infinity of $\Sigma(\Omega)$.
We can imagine $\Sigma(\Omega)$ as follows. Let $\epsilon > 0$. Remove the sets $\{x \in \Omega, |x - v_j| \leq \epsilon\}$ and $\{x \in \Omega, |x - e_k| \leq \epsilon^2\}$. Call the resulting set Ω_ϵ. Then, for ϵ small enough, the closure of Ω_ϵ is diffeomorphic to $\Sigma(\Omega)$.

The example above can be generalized to a curvilinear, stratified polyhedron, using local change of coordinates as in Example 2.9 in 2 dimensions. A detailed construction will be given in Section 4.
A nonstandard example of a curvilinear polyhedral domain is given below.

Example 2.13. We start with a connected polygonal domain $\mathbb{P}$ with connected boundary and we deform it, within the class of connected polygonal domains, until one, and exactly one of the vertices, say A, touches the interior of another edge, say $[B, C]$. (It is clear that such a deformation exists since we allow each side to have arbitrary finite curvature and length.) Let Ω be the resulting connected open set. Then Ω will be a curvilinear polyhedral domain. We define the set $\Sigma(\Omega)$ as for the polygonal domain $\mathbb{P}$, but by introducing polar coordinates in the whole neighborhood of the point A.
If we deform $\mathbb{P}$ to Ω, $\Sigma(\mathbb{P})$ will deform continuously to a space $\Sigma'(\Omega)$, different from $\Sigma(\Omega)$. For certain purposes, the desingularization $\Sigma'(\Omega)$ is better suited than $\Sigma(\Omega)$.

3 Lie manifolds with boundary

The construction of the desingularization $\Sigma(\Omega)$ of a general, curvilinear, stratified polyhedron Ω in n dimensions will be discussed in Section 4. $\Sigma(\Omega)$ will be used both in the definition of weighted Sobolev spaces on the boundary and the proof of a weighted Hardy-Poincaré inequality in Subsection 6.2, which in turn is crucial in establishing coercive estimates for the mixed boundary value/interface problem (6). Since the construction of the desingularization $\Sigma(\Omega)$ relies on properties of manifolds with a Lie structure at infinity, we now recall the definition of a Lie manifold from [2] and of a Lie manifold with boundary from [1], in order to make this paper as self-contained as possible. We also recall a few other needed definitions and results from those papers.

3.1 Definition

We recall that a topological space $\mathfrak{M}$ is, by definition, *a manifold with corners* if every point $p \in \mathfrak{M}$ has a coordinate neighborhood diffeomorphic to $[0,1)^k \times (-1,1)^{n-k}$, $k = 0, 1, \dots, n$, such that the transition functions are smooth (including at the boundary). Given $p \in \mathfrak{M}$, the least integer k with the above property is called the *depth* of p. Since the transition functions are smooth, it therefore makes sense to talk about smooth functions on $\mathfrak{M}$, these being the functions that correspond to smooth functions on $[0,1)^k \times (-1,1)^{n-k}$. We denote by $\mathcal{C}^\infty(\mathfrak{M})$ the set of smooth functions on a manifold with corners $\mathfrak{M}$.

Throughout this paper, $\mathfrak{M}$ will denote a manifold with corners, not necessarily compact. We shall denote by $\mathfrak{M}_0$ the interior of $\mathfrak{M}$ and by $\partial\mathfrak{M} = \mathfrak{M} \smallsetminus \mathfrak{M}_0$ the boundary of $\mathfrak{M}$. The set $\mathfrak{M}_0$ consists of the set of points of depth zero of $\mathfrak{M}$. It is usually no loss of generality to assume that $\mathfrak{M}_0$ is connected. Let $\mathfrak{M}_k$ denote the set of points of $\mathfrak{M}$ of depth k and F_0 be a connected component of $\mathfrak{M}_k$. We shall call F_0 an *open face of codimension* k of $\mathfrak{M}$ and $F := \overline{F}_0$ a *face of codimension* k of $\mathfrak{M}$. A face of codimension 1 will be called a *hyperface* of $\mathfrak{M}$, so that $\partial\mathfrak{M}$ is the union of all hyperfaces of $\mathfrak{M}$. In general, a face of $\mathfrak{M}$ need not be a smooth manifold (with or without corners). A face $F \subset \mathfrak{M}$ which is a submanifold with corners of $\mathfrak{M}$ will be called an *embedded face*.

Anticipating, a Lie manifold with boundary $\mathfrak{M}_0$ is the interior of a manifold with corners $\mathfrak{M}$ together with a Lie algebra of vector fields $\mathcal{V}$ on $\mathfrak{M}$ satisfying certain conditions. To state these conditions, it will be convenient first to introduce a few other concepts.

Definition 3.1. Let $\mathfrak{M}$ be a manifold with corners and $\mathcal{V}$ be a space of vector fields on $\mathfrak{M}$. Let $U \subset \mathfrak{M}$ be an open set and $Y_1, Y_2, \dots, Y_k$ be vector fields on $U \cap \mathfrak{M}_0$. We shall say that $Y_1, Y_2, \dots, Y_k$ form a *local basis of* $\mathcal{V}$ *on* U if the following three conditions are satisfied:

(i) there exist vector fields $X_1, X_2, \dots, X_k \in \mathcal{V}$, $Y_j = X_j$ on $U \cap \mathfrak{M}_0$;

(ii) $\mathcal{V}$ is closed under products with smooth functions in $\mathcal{C}^\infty(\mathfrak{M})$ (*i.e.,* $\mathcal{V} = \mathcal{C}^\infty(\mathfrak{M})\mathcal{V}$) and for any $X \in \mathcal{V}$, there exist smooth functions $\phi_1, \phi_2, \dots, \phi_k \in \mathcal{C}^\infty(\mathfrak{M}_0)$ such that

$$X = \phi_1 X_1 + \phi_2 X_2 + \ldots + \phi_k X_k \quad \text{on } U \cap \mathfrak{M}_0\,; \tag{27}$$

and

(iii) if $\phi_1, \phi_2, \dots, \phi_k \in \mathcal{C}^\infty(\mathfrak{M})$ and $\phi_1 X_1 + \phi_2 X_2 + \ldots + \phi_k X_k = 0$ on $U \cap \mathfrak{M}_0$, then $\phi_1 = \phi_2 = \ldots = \phi_k = 0$ on U.

We now recall structural Lie algebras of vector fields from [2].

Definition 3.2. A subspace $\mathcal{V} \subseteq \Gamma(\mathfrak{M}, T\mathfrak{M})$ of the Lie algebra of all smooth vector fields on $\mathfrak{M}$ is said to be a *structural Lie algebra of vector fields on* $\mathfrak{M}$ provided that the following conditions are satisfied:

(i) $\mathcal{V}$ is closed under the Lie bracket of vector fields;

(ii) every vector field $X \in \mathcal{V}$ is tangent to all hyperfaces of $\mathfrak{M}$;

(iii) $\mathcal{C}^\infty(\mathfrak{M})\mathcal{V} = \mathcal{V}$; and

(iv) for each point $p \in \mathfrak{M}$ there exist a neighborhood U_p of p in $\mathfrak{M}$ and a local basis of $\mathcal{V}$ on U_p.

The concept of Lie structure at infinity, defined next, is also taken from [2].

Definition 3.3. A *Lie structure at infinity* on a smooth manifold $\mathfrak{M}_0$ is a pair $(\mathfrak{M}, \mathcal{V})$, where $\mathfrak{M}$ is a compact manifold, possibly with corners, and $\mathcal{V} \subset \Gamma(\mathfrak{M}, T\mathfrak{M})$ is a structural Lie algebra of vector fields on $\mathfrak{M}$ with the following properties:

(i) $\mathfrak{M}_0 = \mathfrak{M} \setminus \partial\mathfrak{M}$, the interior of $\mathfrak{M}$, and

(ii) If $p \in \mathfrak{M}_0$, then any local basis of $\mathcal{V}$ in a neighborhood of p is also a local basis of the tangent space to $\mathfrak{M}_0$. (In particular, the constant k of Equation (27) equals n, the dimension of $\mathfrak{M}_0$.)

A *manifold with a Lie structure at infinity* (or, simply, a *Lie manifold*) is a manifold $\mathfrak{M}_0$ together with a Lie structure at infinity $(\mathfrak{M}, \mathcal{V})$ on $\mathfrak{M}_0$. We shall sometimes denote a Lie manifold as above by $(\mathfrak{M}_0, \mathfrak{M}, \mathcal{V})$, or, simply, by $(\mathfrak{M}, \mathcal{V})$, because $\mathfrak{M}_0$ is determined as the interior of $\mathfrak{M}$.
Let $\mathcal{V}_b$ be the set of vector fields on $\mathfrak{M}$ that are tangent to all faces of $\mathfrak{M}$. Then $(\mathfrak{M}, \mathcal{V}_b)$ is a Lie manifold [57]. See [1, 2, 47] for more examples.

3.2 Riemannian metric

Let $(\mathfrak{M}, \mathcal{V})$ be a Lie manifold and g a Riemannian metric on $\mathfrak{M}_0 := \mathfrak{M} \setminus \partial\mathfrak{M}$. We shall say that *$g$ is compatible* (with the Lie structure at infinity $(\mathfrak{M}, \mathcal{V})$) if, for any $p \in \mathfrak{M}$, there exist a neighborhood U_p of p in $\mathfrak{M}$ and a local basis $X_1, X_2, \ldots, X_n$ of $\mathcal{V}$ on U_p that is orthonormal with respect to g on U_p.
It was proved in [2] that $(\mathfrak{M}_0, g_0)$ is necessarily of infinite volume and complete. Moreover, all the covariant derivatives of the Riemannian curvature tensor of g are bounded.
We also know that the injectivity radius is bounded from below by a positive constant, *i.e.,* $(\mathfrak{M}_0, g_0)$ is of bounded geometry [18]. (A *manifold with bounded geometry* is a Riemannian manifold with positive injectivity radius and with bounded covariant derivatives of the curvature tensor, see for example [16] or [69] and references therein).

3.3 $\mathcal{V}$-differential operators

We are especially interested in the analysis of the differential operators generated using only derivatives in $\mathcal{V}$. Let $\mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M})$ be the algebra of differential operators on $\mathfrak{M}$ generated by multiplication with functions in $\mathcal{C}^\infty(\mathfrak{M})$ and by differentiation with vector fields $X \in \mathcal{V}$. The space of order m differential operators in $\mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M})$ will be denoted $\mathrm{Diff}^m_{\mathcal{V}}(\mathfrak{M})$. A differential operator in $\mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M})$ will be called a $\mathcal{V}$-differential operator. We define the set $\mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M}; E, F)$ of $\mathcal{V}$-differential operators acting between sections of smooth vector bundles $E, F \to \mathfrak{M}$ in the usual way [1, 2].
A simple but useful property of the differential operator in $\mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M})$ is that

$$x^s P x^{-s} \in \mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M}) \tag{28}$$

for any $P \in \mathrm{Diff}^*_{\mathcal{V}}(\mathfrak{M})$ and any defining function x of some hyperface of $\mathfrak{M}$ [3]. This property is easily proved using the fact that X is tangent to the hyperface defined by x, for any $X \in \mathcal{V}$ (a proof of a slightly more general fact is included in Corollary 6.3).

3.4 Lie manifolds with boundary

A subset $\mathfrak{N} \subset \mathfrak{M}$ is called a *submanifold with corners of* $\mathfrak{M}$ if $\mathfrak{N}$ is a closed submanifold of $\mathfrak{M}$ such that $\mathfrak{N}$ is transverse to all faces of $\mathfrak{M}$ and any face of $\mathfrak{N}$ is a component of $\mathfrak{N} \cap F$ for some face F of $\mathfrak{M}$.
The following definition is a reformulation of a definition of [1].

Definition 3.4. Let $(\mathfrak{N}, \mathcal{W})$ and $(\mathfrak{M}, \mathcal{V})$ be Lie manifolds, where $\mathfrak{N} \subset \mathfrak{M}$ is a submanifold with corners and

$$\mathcal{W} = \{X|_{\mathfrak{N}},\, X \in \mathcal{V}, X|_{\mathfrak{N}} \text{ tangent to } \mathfrak{N}\}.$$

We shall say that $(\mathfrak{N}, \mathcal{W})$ is a *tame* submanifold of $(\mathfrak{M}, \mathcal{V})$ if, for any $p \in \partial\mathfrak{N}$ and any $X \in T_p\mathfrak{M}$, there exist $Y \in \mathcal{V}$ and $Z \in T_p\mathfrak{N}$ such that $X = Y(p) + Z$.

Let $\mathfrak{N} \subset \mathfrak{M}$ be a submanifold with corners. We assume that $\mathfrak{M}$ and $\mathfrak{N}$ are endowed with the Lie structures $(\mathfrak{N}, \mathcal{W})$ and $(\mathfrak{M}, \mathcal{V})$. We shall say that $\mathfrak{N}$ is a *regular* submanifold of $(\mathfrak{M}, \mathcal{V})$ if we can choose a tubular neighborhood V of $\mathfrak{N}_0 := \mathfrak{N} \smallsetminus \partial\mathfrak{N} = \mathfrak{N} \cap \mathfrak{M}_0$ in $\mathfrak{M}_0$, a compatible metric g_1 on $\mathfrak{N}_0$, a product-type metric g_1 on V that reduces to g_1 on $\mathfrak{N}_0$, and a compatible metric on $\mathfrak{M}_0$ that restricts to g_1 on V. Theorem 5.8 of [2] states that every tame submanifold is regular. The point of this result is that it is much easier to check that a submanifold is tame than to check that it is regular.
In the case when $\mathfrak{N}$ is of codimension one in $\mathfrak{M}$, the condition that $\mathfrak{N}$ be tame is equivalent to the fact that there exists a vector field $X \in \mathcal{V}$ that restricts to a normal vector of $\mathfrak{N}$ in $\mathfrak{M}$. The neighborhood V will then be of the form $V \simeq (\partial\mathfrak{N}_0) \times (-\varepsilon_0, \varepsilon_0)$. Moreover, there will exist a compatible metric on $\mathfrak{M}_0$ that restricts to the product metric $g_1 + dt^2$ on V, where g_1 is a compatible metric on $\mathfrak{N}_0$.

Let A be a subset of $\mathfrak{M}$. We denote by $\partial_{\mathfrak{M}} A := \overline{A} \smallsetminus A$ the boundary of A computed within $\mathfrak{M}$, which should not be confused with $\partial A = A \smallsetminus A_0$, where A_0 is the interior of A, as a manifold with corners. Let $\mathbb{D} \subset \mathfrak{M}$ be an open subset. We say that $\mathbb{D}$ is a *Lie domain* in $\mathfrak{M}$ if, and only if,

$$\partial_{\mathfrak{M}} \mathbb{D} = \partial_{\mathfrak{M}} \overline{\mathbb{D}} \tag{29}$$

and $\partial_{\mathfrak{M}} \mathbb{D}$ is a regular submanifold of $\mathfrak{M}$. The condition (29) is included in order to make sure that $\mathbb{D}$ is on only one side of its boundary. A typical example of a Lie domain $\mathbb{D} \subset \mathfrak{M}$ is obtained by considering a regular submanifold with corners $\mathfrak{N} \subset \mathfrak{M}$ of codimension one with the property that $\mathfrak{M} \smallsetminus \mathfrak{N}$ consists of two connected components. Any of these two components will be a Lie domain.

Definition 3.5. A *Lie manifold with boundary* is a triple $(\mathfrak{O}_0, \mathfrak{O}, \mathcal{V}')$, where $\mathfrak{O}_0$ is a smooth manifold with boundary, $\mathfrak{O}$ is a compact manifold with corners containing $\mathfrak{O}_0$ as an open subset, and $\mathcal{V}'$ is a Lie algebra of vector fields on $\mathfrak{O}$ with the property that there exists a Lie manifold $(\mathfrak{M}_0, \mathfrak{M}, \mathcal{V})$, a Lie domain $\mathbb{D}$ in $\mathfrak{M}$ and a diffeomorphism $\phi : \mathfrak{O} \to \overline{\mathbb{D}}$ such that $\phi(\mathfrak{O}_0) = \overline{\mathbb{D}} \cap \mathfrak{M}_0$ and $D\phi(\mathcal{V}|_{\mathbb{D}}) = \mathcal{V}'$.

We continue with some simple observations. First note that if $(\mathfrak{O}_0, \mathfrak{O}, \mathcal{V})$ is a Lie manifold with boundary, then $\mathfrak{O}_0$ is determined by $(\mathfrak{O}, \mathcal{V})$. Indeed, if we remove from $\mathfrak{O}$ the hyperfaces H with the property that $\mathcal{V}$ consists only of vectors tangent to H, then the resulting set is $\mathfrak{O}_0$. Therefore, we can denote the Lie manifold with boundary $(\mathfrak{O}_0, \mathfrak{O}, \mathcal{V})$ simply by $(\mathfrak{O}, \mathcal{V})$.
Another observation is that $\partial \mathfrak{O}_0$, the boundary of $\mathfrak{O}_0$ (as a smooth manifold with boundary), has a canonical structure of Lie manifold $(\partial \mathfrak{O}_0, D = \partial_{\mathfrak{M}} \mathbb{D}, \mathcal{W})$, where $\mathcal{W} = \{X|_D,\, X \in \mathcal{V}, X|_D \text{ is tangent to } D\}$. The compactification D is the closure of $\partial \mathfrak{O}_0$ in $\mathfrak{O}$.

3.5 Sobolev spaces

The main reason for considering Lie manifolds (with or without boundary) in our setting is that they carry some naturally defined Sobolev spaces and these Sobolev spaces behave almost exactly like the Sobolev spaces on a compact manifold with a smooth boundary. Let us recall one of the equivalent definitions in [1]. See also [16, 32, 57, 64, 70] for results on Sobolev spaces on non-compact manifolds.

Definition 3.6. Fix a Lie manifold $(\mathfrak{M}, \mathcal{V})$. The spaces $L^2(\mathfrak{M}_0) = L^2(\mathfrak{M}_0)$ are defined using the natural volume form on $\mathfrak{M}_0$ given by an arbitrary compatible metric g on $\mathfrak{M}_0$ (*i.e.,* compatible with the Lie structure at infinity). All such volume forms are known to define the same space $L^2(\mathfrak{M})$, but with possibly different norms. Let $k \in \mathbb{Z}_+$. Choose a finite set of vector fields $\mathcal{X} \subset \mathcal{V}$ such that $\mathcal{C}^\infty(\mathfrak{M})\mathcal{X} = \mathcal{V}$. The system $\mathcal{X}$ gives rise to the norm

$$\|u\|^2_{\mathcal{X},\Omega} := \sum \|X_1 X_2 \dots X_\mu u\|^2_{L^2(\Omega)}\,, \quad 1 \leq p < \infty, \tag{30}$$

the sum being over all possible choices of $0 \leq l \leq k$ and all possible choices of vector fields $X_1, X_2, \ldots, X_l \in \mathcal{X}$, not necessarily distinct. We then set

$$H^k(\mathfrak{M}_0) = H^k(\mathfrak{M}) := \{u \in L^2(\mathfrak{M}),\ \|u\|_{\mathcal{X},\mathfrak{M}} < \infty\}.$$

The spaces $H^s(\mathfrak{M}_0) = H^s(\mathfrak{M})$ are defined by duality (with pivot $L^2(\mathfrak{M}_0)$) when $-s \in \mathbb{Z}_+$, and then by interpolation, as above.
Let $(\mathfrak{D}_0, \mathfrak{D}, \mathcal{V})$ be a Lie manifold with boundary. We shall assume that $\mathfrak{D}$ is the closure of a Lie domain $\mathbb{D}$ of the Lie manifold $\mathfrak{M}$. The Sobolev spaces $H^k(\mathfrak{D}_0)$ are defined as the set of *restrictions* to $\mathfrak{D}_0$ of distributions $u \in H^k(\mathfrak{M}_0)$, using the notation of Definition 3.5, $k \in \mathbb{Z}$. In particular, we obtain the following description of $H^k(\mathfrak{D}_0)$ from [1].

Lemma 3.7. *We have, for $k \geq 0$,*

$$H^k(\mathfrak{D}_0) = \{u \in L^2(\mathfrak{D}_0),\ \|u\|_{\mathcal{X}} < \infty\},$$

and

$$H^{-k}(\mathfrak{D}_0) = H^k_0(\mathfrak{D}_0)^*,$$

where $H^k_0(\mathfrak{D}_0)$ is the closure of $\mathcal{C}^\infty_c(\mathfrak{D}_0)$ in $H^k(\mathfrak{M}_0)$.

Definition 3.8. The hyperfaces of $\mathfrak{D}$ that do not intersect the boundary $\partial\mathfrak{D}_0$ of the manifold with boundary $\mathfrak{D}_0$ will be called *hyperfaces at infinity*. Let x_H be a defining function of the hyperface H of $\mathfrak{D}$. Any function of the form $h = \prod x_H^{a_H}$, where H ranges through the set of hyperfaces at infinity of $\mathfrak{D}$ and $a_H \in \mathbb{R}$, will be called an *admissible weight*. If h is an admissible weight, we set

$$hH^\mu(\mathfrak{D}_0) = \{h\,u;\ u \in H^\mu(\mathfrak{D}_0)\}$$

with the induced norm.

Later in the paper, we will identify the weighted Sobolev spaces $\mathcal{K}^s_a(\Omega)$ with suitable spaces $hH^s(\mathfrak{D}_0)$ in Proposition 5.7 and utilize the spaces $hH^s(\partial\mathfrak{D}_0)$ to define the spaces $\mathcal{K}^s_a(\partial\Omega)$ on the boundary in Definition 5.8, for Ω a curvilinear, stratified polyhedral domain in dimension n. The following proposition, which summarizes the relevant results from Theorem 3.4 and 3.7 from [1], will then imply Theorem 5.9.

Proposition 3.9. *The restriction to the boundary extends to a continuous, surjective map $hH^\mu(\mathfrak{D}_0) \to hH^{\mu-1/2}(\partial\mathfrak{D}_0)$, for any $\mu \geq 1$ and any admissible weight h. The kernel of this map, for $\mu = 1$, consists of the closure of $\mathcal{C}^\infty_c(\mathfrak{D}_0)$ in $hH^1(\mathfrak{D}_0)$.*

For $\mathbb{D}$, $\mathfrak{D}$, $\mathfrak{D}_0$ as in the proposition above, $hH^s(\mathbb{D})$, $hH^s(\mathfrak{D})$, and $hH^s(\mathfrak{D}_0)$ will all denote the same space.

4 Desingularization of polyhedra

In this section, we introduce a desingularization procedure that we shall use for studying curvilinear polyhedral domains. The desingularization will carry a natural structure of Lie manifold with boundary. This construction will allow us to study curvilinear polyhedral domains using Lie manifolds with boundary. The desingularization of a domain $\Omega \subset M$ depends on M in general (since $\overline{\Omega}$ depends on M), but we do not include the dependence on M in the notation, and generally ignore this issue in order to streamline the presentation, since the manifold M will be clear from the context in most cases.
As before, $\Omega \subset M$ denotes a curvilinear, stratified polyhedral domain in an n-dimensional manifold M. We shall construct by induction on n a *canonical* manifold with corners $\Sigma(\Omega)$ and a differentiable map $\kappa : \Sigma(\Omega) \to \overline{\Omega}$ that is a diffeomorphism from the interior of $\Sigma(\Omega)$ to Ω. In particular, the map κ allows us to identify Ω with a subset of $\Sigma(\Omega)$. We shall also construct a canonical Lie algebra of vector fields $\mathcal{V}(\Omega)$ on $\Sigma(\Omega)$. The manifold $\Sigma(\Omega)$ will be called the *desingularization of* Ω, the map κ will be called the *desingularization* map, and the Lie algebra of vector fields will be called the *structural Lie algebra of vector fields of* $\Sigma(\Omega)$. We shall also introduce in this section a smooth weight function r_Ω equivalent to η_{n-2}.
The space $\Sigma(\Omega)$ that we construct is not optimal if the links ω_p are not connected. A better desingularization would be obtained if one considers a diffeomorphism ϕ_{pC} for each connected component C of $V_p \cap \Omega$ that maps C to a conic set of the form $\omega_{p,C} \times B^\lambda$, with λ largest possible. The difference between these two constructions is seen by looking at the Example 2.13.

Notations 4.1. *From now on V_p and $\phi_p : V_p \to tB^{n-l} \times tB^l$, $l = \ell(p)$, will denote a neighborhood of $p \in \partial\Omega$ in $M \supset \Omega$ and ϕ_p will be a diffeomorphism satisfying the conditions of Definition* (2.1). *In addition, $\omega_p \subset S^{n-l-1}$ will be the curvilinear, stratified polyhedron such that*

$$\phi_p(V_p \cap \Omega) = \{(rx', x'')\},\ r \in (0,t), x' \in \omega_p \text{ and } x'' \in tB^l\},$$

i.e., *ω_p is the link of Ω at p. This notation will remain fixed throughout the paper.*

Recall that $0 \leq \ell(p) \leq n-1$ is defined to be the smallest integer such that $p \in \Omega^{(\ell(p))}$, but $p \notin \Omega^{(\ell(p)-1)}$. If $\ell(p) = 0$, then B^l is reduced to a point, and we just drop x'' from the notation above. We will assume that ϕ_p extends to the closure of V_p, if necessary.

4.1 The desingularization $\Sigma(\Omega)$

We now define the canonical desingularization of a curvilinear polyhedral domain $\Omega \subset M$, M an n-dimensional smooth manifold. For $n = 0$, Ω consists of finitely many points. Then we define $\Sigma(\Omega) = \Omega$ and $\kappa = id$. To define $\Sigma(\Omega)$ for general Ω, we shall proceed by induction.

We need first to make the important observation that the set ω_p, $p \in \partial\Omega$, of Definition 2.1 is determined up to a linear isomorphism of $\mathbb{R}^{n-l-1}$. Indeed, let $S_p \subset \partial\Omega$ be the maximal connected manifold of dimension $l = \ell(p)$ passing through p that is, the connected component of $\Omega^{(l)} \smallsetminus \Omega^{(l-1)}$ containing p. Let $(T_pS_p)^\perp = T_pM/T_pS_p$. The differential $D\phi_p : T_pM \to \mathbb{R}^n = T_0\mathbb{R}^n$ of the map ϕ_p at p has then the property that $D\phi_p(T_pS_p) = T_0\mathbb{R}^l$, $D\phi_p\big((T_pS_p)^\perp\big) = T_0\mathbb{R}^n/T_0\mathbb{R}^l = \mathbb{R}^{n-l}$. We will define a canonical set $\mathcal{N}_p \subset (T_pS_p)^\perp$ such that

$$D\phi_p(\mathcal{N}_p) \simeq \mathbb{R}_+\omega_p.$$

Since the definition of $\mathcal{N}_p$, which we give next, is independent of any choices used in the definition of a polyhedral domain, it follows that ω_p is unique, up to a linear isomorphism of $\mathbb{R}^{n-l-1}$. It remains to define the set $\mathcal{N}_p$ with the desired independence property. It is enough to define the *complement* of $\mathcal{N}_p$. This complement is the projection onto $(T_pS_p)^\perp = T_pM/T_pS_p$ of the set $\gamma'(0) \in T_pM$, where γ ranges through the set of smooth curves $\gamma : [0,1] \to M$, with $\gamma(t) \notin \Omega$ for $t > 0$, and $\gamma(0) = p$.

We let then $\sigma_p := \mathcal{N}_p/\mathbb{R}_+$, the set of rays in $\mathcal{N}_p$, for $p \in \partial\Omega$. Any choice of a metric on $T_pM/T_pS_p \supset \mathcal{N}_p$ will identify σ_p with a subset of the unit sphere of T_pM/T_pS_p, which depends however on the metric. In particular, $D\phi_p : \sigma_p \to \omega_p$ is a diffeomorphism. If p is not in the singular set $\Omega^{(n-2)}$ of Ω, then σ_p consists exactly of one point. The map κ is the projection onto the second component and is one-to-one above Ω and above $\Omega^{(n-1)} \smallsetminus \Omega^{(n-2)} \subset \partial\Omega$.

We now proceed with the induction step. Assume $\Sigma(\omega)$ and $\kappa : \Sigma(\omega) \to \overline{\omega}$ have been constructed for all curvilinear, stratified polyhedral domains ω of dimension at most $n-1$. If $p \in \Omega$, we then set $\sigma_p = \{0\} = \Sigma(\sigma_p)$. Let Ω be an arbitrary curvilinear, stratified polyhedral domain of dimension n. We define

$$\Sigma(\Omega) := \bigcup_{p\in\Omega} \{p\} \times \Sigma(\sigma_p) = \Omega \cup \bigcup_{p\in\partial\Omega} \{p\} \times \Sigma(\sigma_p). \tag{31}$$

In particular, if Ω is a bounded domain with smooth boundary, then $\Sigma(\Omega) \simeq \Omega$. This definition is consistent as ω_p is a curvilinear polyhedral domain of dimension at most $n-1$. Below, an open embedding will mean a diffeomorphism onto an open subset of the codomain.

Proposition 4.2. *Let $\Omega \subset M$ and $\Omega' \subset M'$ be curvilinear, stratified polyhedral domains and $\Phi : M \to M'$ be an open embedding such that $\Phi(\Omega)$ is a union of connected components of $\Omega' \cap \Phi(M)$. Then the embedding Φ defines a canonical map $\Sigma(\Phi) : \Sigma(\Omega) \to \Sigma(\Omega')$ such that*

$$\Sigma(\Phi \circ \Phi') = \Sigma(\Phi) \circ \Sigma(\Phi'),$$

for all open embeddings Φ and Φ' for which $\Sigma(\Phi \circ \Phi')$, $\Sigma(\Phi) \circ \Sigma(\Phi')$ are well-defined.

Proof. The proof is by induction. There is nothing to prove for $n = 0$. Let $p \in \overline{\Omega}$. We have that $\Phi(\overline{\Omega}) \subset \overline{\Omega'}$, and hence $\Phi(p) \in \overline{\Omega'}$, as well. Let V_p' be an

open neighborhood of $\Phi(p)$ in M' such that there exists a diffeomorphism $\phi'_p : V'_p \to B^{n-l} \times B^l$ satisfying the condition (18) of the definition of a polyhedral domain (*i.e.,* $\phi'_p(\Omega' \cap V'_p)$ is $\mathbb{R}_+\omega'_p \times B^l$, for some curvilinear polyhedral domain $\omega'_p \subset S^{n-l-1}$). By decreasing V'_p, if necessary, we can assume that $V'_p \subset \Phi(M)$. Then $V'_p \cap \Phi(\Omega)$ is a union of connected components of $V'_p \cap \Omega'$. Therefore ω'_p is a union of connected components of $\Phi(\omega_p)$, where $\omega_p \subset S^{n-l-1}$ is associated to $p \in \overline{\Omega}$ in the same way as ω'_p was associated to $\Phi(p) \in \overline{\Omega'}$. The induction hypothesis then gives rise to a canonical, injective map $\Sigma(\omega_p) \to \Sigma(\omega'_p)$. The map $\Sigma(\Phi)$ is obtained by combining these different maps.
The functoriality (*i.e.,* the relation $\Sigma(\Phi\circ\Phi') = \Sigma(\Phi)\circ\Sigma(\Phi')$) is proved similarly by induction. □

Here is a corollary of the above proof.

Corollary 4.3. *If $\Omega = \Omega' \cup \Omega''$ is the disjoint union of two open sets, then the inclusions $\Sigma(\Omega') \subset \Sigma(\Omega)$ and $\Sigma(\Omega') \subset \Sigma(\Omega)$ defined in Proposition 4.2 realize $\Sigma(\Omega) = \Sigma(\Omega') \cup \Sigma(\Omega'')$, where the union is a disjoint union.*

Proof. We use the same argument as in the proof of Proposition 4.2. □

The desingularization has a simple behavior with respect to products.

Lemma 4.4. *We have a canonical identification*

$$\Sigma(M' \times \Omega) = M' \times \Sigma(\Omega),$$

for any smooth manifolds M and M' and any curvilinear polyhedral domain $\Omega \subset M$.

Proof. Since M' is smooth, we can choose the structural local diffeomorphism $\phi_{(p,q)}$ in $M' \times \Omega$ to be given by $\phi_p \times \psi_q$, where ψ_p is a local coordinate chart defined in a neighborhood of $p \in M'$ and ϕ_q is the local diffeomorphism of a neighborhood of q in Ω. Indeed, then

$$\Sigma(M' \times \Omega) := \cup_{p,q}\{(p,q)\} \times \Sigma(\sigma_{(p,q)}) = \cup_{p,q}\{(p,q)\} \times \Sigma(\sigma_q) = M' \times \Sigma(\Omega), \quad (32)$$

where $q \in \overline{\Omega}$ and $p \in M'$. Consequently, there is a canonical bijection $\sigma_{(p,q)} \simeq \sigma_q$ for any $q \in \overline{\Omega}$ and any $p \in M'$ (so (p,q) is in the closure of $M' \times \Omega$ in $M' \times M$). □

It remains to define the topology and differentiable structure on $\Sigma(\Omega)$. These definitions will again be canonical if we require that the map of the above lemma, as well as the maps κ and $\Sigma(\phi)$, be differentiable, for any open embedding ϕ.
Let $V_p \subset M$ and ϕ_p be as in Equation (19). By Proposition 4.2, we may assume that ϕ_p is the identity, so that $p = 0$, $V_p = B^{n-l} \times B^l$, and $V_p \cap \Omega = I\omega_p \times B^l$, with $I = (0,1)$. Let $(\Sigma(\omega_p), \kappa'_p)$ be the canonical desingularization of ω_p in S^{n-l-1}. We shall need the following lemma.

Lemma 4.5. *We have a canonical identification*

$$\Sigma(V_p \cap \Omega) = [0,1) \times \Sigma(\omega_p) \times B^l$$

such that the desingularization map

$$\kappa_p : [0,1) \times \Sigma(\omega_p) \times B^l \to \overline{V_p \cap \Omega} \subset B^{n-l} \times B^l$$

is given by $\kappa_p(r, x', y) = (r\kappa_p'(x'), y)$.

Proof. We may assume $p = 0$. Let $I = (0,1)$. The closure of $V_0 \cap \Omega$ in $V_0 = V_p$ is the disjoint union $\{0\} \times B^l \cup I\overline{\omega}_0 \times B^l$. Accordingly, we decompose $\Sigma(V_0 \cap \Omega, M)$ into two disjoint sets, corresponding to this splitting of the closure of $V_0 \cap \Omega$. Recall that by definition $\Sigma(V_0 \cap \Omega)$ is the union $\cup_{p \in \overline{V_0 \cap \Omega}} \{p\} \times \Sigma(\sigma_p)$. Using also Lemma 4.4, we then obtain

$$\begin{aligned}\Sigma(V_0 \cap \Omega) = \Sigma(V_0 \cap \Omega) \cup \bigcup_{q \in B^l} \{(0,q)\} \times \Sigma(\omega_0) \\ = \Sigma((0,1) \times \omega_0 \times B^l) \cup \bigcup_{q \in B^l} \{(0,q)\} \times \Sigma(\omega_0) \\ = (0,1) \times \Sigma(\omega_0) \times B^l \cup \{0\} \times \Sigma(\omega_0) \times B^l = [0,1) \times \Sigma(\omega_0) \times B^l.\end{aligned}$$

The formula for κ_0 follows from the definition. □

Since $\Sigma(\Omega)$ is the union of all the sets $\Sigma(V_p \cap \Omega)$, with V_p in the covering above, we can define the topology and smooth structure on $\Sigma(\Omega)$ by induction as follows (there is nothing to define in the case Ω has dimension zero, since then $\Sigma(\Omega) = \Omega$).

Definition 4.6. Let $\phi_p : V_p \to B^{n-l} \times B^l$ and ω_p be as in Definition 2.1. The topology and smooth structure on $\Sigma(\Omega)$ are such that the induced structure on $\Sigma(V_p \cap \Omega)$ is the same as the one obtained from the canonical identification $\Sigma(V_p \cap \Omega) = [0,1) \times \Sigma(\omega_p) \times B^l$ of Lemma 4.5.

The smooth structure on $\Sigma(\Omega)$ is therefore defined using a covering with sets of the form $\Sigma(V_p \cap \Omega)$ (this desingularization is with respect to V_p and not $M \subset \Omega$!). We need to prove that the transition functions are smooth. This property follows from the fact that the maps ϕ_p are diffeomorphisms and from Lemma 4.5.
We have therefore completed the definition of the desingularization $\Sigma(\Omega)$ and of its smooth structure.

4.2 The distance to singular boundary points

We continue with a study of the geometric and, especially, metric properties of $\Sigma(\Omega)$. We first argue that $\Sigma(\Omega)$ has embedded faces and hence that every hyperface of $\Sigma(\Omega)$ has a defining function.

Let F_0 be an open hyperface of a manifold with corners $\mathfrak{M}$. Then F_0 is a manifold of dimension $n-1$. Its closure F, in general, will not necessarily be a manifold, because it may have self-intersections. (A typical example is the boundary of a curvilinear polygonal domain with only one vertex, the "tear drop domain.") By induction, however, it follows that $F_0 \cap V_p$ will be a manifold with corners, for any p. In particular, we obtain that all (closed) faces of $\Sigma(\Omega)$ are embedded submanifolds of $\Sigma(\Omega)$. Let H be a hyperface of $\Sigma(\Omega)$, since H is an embedded submanifold of codimension 1, there will exist a function $x_H > 0$ on Ω, $H = \{x_H = 0\}$, and $dx_H \neq 0$ on H. A function x_H with this property is called a *defining function of* H [57].

One of the main reasons for introducing the desingularization space $\Sigma(\Omega)$ is the following result.

Proposition 4.7. *Let Ω be a bounded, curvilinear, stratified polyhedral domain and g_1 and g_2 be two smooth Riemannian metrics on M. Let us fix k and assume $\Omega^{(k)} \neq \emptyset$. Let $f_j(x)$ be the modified distance from $x \in \overline{\Omega}$ to the set $\Omega^{(k)}$ in the metric g_j, computed within $\overline{\Omega}$. Then the quotient f_2/f_1 extends to a continuous function on $\Sigma(\Omega)$.*

Proof. It is enough to prove the given property in the neighborhood of every point $p \in \overline{\Omega}$. So let us fix $p \in \overline{\Omega}$. By replacing V_p with a smaller neighborhood of p, if necessary, we can also assume that $g_2(\xi) \leq Cg_1(\xi)$, which implies that $f_2 \leq Cf_1$, and hence that f_2/f_1 is bounded.

We shall prove the statement by induction on n. In the case $n = 1$, the only possibility is that $k = 0$, or otherwise $\Omega^{(k)} = \emptyset$. Then $f(x)$ is the distance to the vertices of Ω. Recall that Ω is a disjoint union of open intervals in this case, so that we can reduce to consider a single interval. If say $\Omega = [a, b]$, then close to a, $f_j(x) = a_j(x)(x-a)$, with a_j smooth near a and $a_j(a) \neq 0$. The same situation holds at b. This proves our result in the case $n = 1$. We now proceed with the induction step.

The function f_1/f_2 is clearly continuous on the open set Ω. Fix $p \in \partial\Omega$. We shall construct an open neighborhood U_p of p in $\overline{\Omega}$ such that f_1/f_2 extends to a continuous function on $\kappa^{-1}(U_p)$. Let V_p be as in the definition of polyhedral domains (Definition 2.1). We shall identify $V_p \cap \Omega$ with $I\omega_p \times B^l$ using the diffeomorphism ϕ_p of Equation (19). If $l > k$, that is, $p \in \Omega^{(l)} \smallsetminus \Omega^{(k)}$, then both f_1 and f_2 extend to continuous, non-vanishing functions on $V_p \cap \overline{\Omega}$, which can be lifted to continuous, non-vanishing functions on $\kappa^{-1}(V_p \cap \Omega)$. We shall assume hence that $k \geq l$.

On a smaller neighborhood $V' \subset V_p$, if necessary, we can arrange that the function f_1 gives the distance to $V_p^{(k)}$, that is, that the point of $\Omega^{(k)}$ closest to $x \in V' \cap \Omega$ is, in fact, in V_p. By decreasing V' even further, we can further arrange that the same holds for f_2. Then we shall take $U_p := V'$.

To prove that f_2/f_1 extends to a continuous function on $\kappa^{-1}(U_p)$, it is enough to do that in the case $\Omega = V_p \cap \Omega$, because the quotient f_2/f_1 does not change on $U_p \cap \Omega$ if we replace Ω with $V_p \cap \Omega$, as explained in the paragraph above. We can also assume that g_2 is the standard Euclidean metric, but then we have to prove that f_1/f_2 extends to a *nowhere vanishing* continuous function on $\Sigma(\Omega)$. (Using also Proposition 4.2, we have reduced to the case $\Omega = I\omega_p \times B^l \subset \mathbb{R}^n$, $I = (0,t)$.)

The scaling property of the Euclidean metric and our assumption that $k \geq l$ imply that

$$f_2(rx', x'') = rf_2(x', x''),$$

for any $r \in [0,1]$. Let g_0 be a constant metric on $\mathbb{R}^n$ that coincides with g_1 at the origin.

Let f_0 be associated to g_0 in the same way as f_j is associated to g_j, for $j = 1, 2$, *i.e.,* $f_0(x) = \operatorname{dist}(x, \Omega^{(k)})$ using the metric g_0. We then have similarly $f_0(rx', x'') = rf_0(x', x'')$, so that the quotient $f_0(rx', x'')/f_1(rx', x'')$ does not depend on r. We can therefore fix $r = 1$. Consequently, we can work with the lower dimensional polyhedral domain $\omega := \omega_p \times B^l$ instead of $\Omega = I\omega_p \times B^l$, and prove that f_0/f_1 extends by continuity to $\Sigma(\omega)$. It remains to see that we can use induction to prove the existence of this extension. Since ω is by construction a stratified polyhedron, we denote by $\omega^{(k)} = \omega^{(k)} \times B^l$ $k < n$, its associated stratification, where we set $\omega_p^{(k-l-1)} = \emptyset$ if $k - l - 1 < 0$ as before. Let f_1' be the distance function to $\omega^{(k-1)}$ on ω (*i.e.,* computed *within* $\overline{\omega}$, with respect to the metric induced by g_1, as in the statement of Proposition 4.7). We let $f_1' = 1$ if $\omega_p^{(k-l-1)} = \emptyset$.

We define f_0' similarly. The inductive hypothesis guarantees that f_0'/f_1' extends to a continuous function on $\Sigma(\omega) = \Sigma(\omega_p) \times B^l$. On the other hand, it is easy to see that both f_1/f_1' and f_1'/f_1 extend to continuous functions on $\overline{\omega}$ if we set them to be equal to 1 on $\omega^{(k-1)}$. The same is true of f_0/f_0' and f_0'/f_0. Putting all these estimates together, it follows that

$$f_0/f_1 = (f_0/f_0')(f_0'/f_1')(f_1'/f_1)$$

extends to a continuous, nowhere vanishing function on $\Sigma(\omega)$.

Let us tackle now the case g_2 arbitrary. Let f_0 be defined as before. We then have that $f_2(rx', x'') = rf_0(x', x'') + r^2 h(rx', x'')$, with h a continuous function on $\Sigma(V_p \times \Omega)$ that vanishes on $\Omega^{(k)}$. Then

$$\frac{f_2}{f_1} = \frac{f_0}{f_1} + r\frac{h(rx', x'')}{f_1(x', x'')}.$$

The function f_0/f_1 was already shown to extend by continuity to $\Sigma(\Omega)$. The same argument as above shows that h/f_1 extends by continuity to a nowhere vanishing function on

$$[\epsilon, 1) \times \Sigma(\omega_p) \times B^l \subset [0,1) \times \Sigma(\omega_p) \times B^l =: \Sigma(\Omega).$$

The continuity of f_2/f_1 then follows from the boundedness of f_2/f_1.

The resulting function does not vanish at $r = 0$, because it is equal to f_0/f_1 there. It was already proved that it does not vanish for $\epsilon > 0$. The proof is complete. □

We shall need also the following corollary of the above proof.

Corollary 4.8. *Identify $V_p \cap \Omega = \Omega$ with $I\omega_p \times B^l$, $I = (0, a)$, $l = \ell(p)$, using the diffeomorphism ϕ_p given in Definition 2.1. Let g be a smooth metric on V_p, and let $f(x)$ be the distance from x to $\Omega^{(k)}$, $k \geq l$, $f'(x', x'')$ be the distance from $(x', x'') \in \omega := \omega_p \times B^l$ to $\omega^{(k-1)}$ (within $\overline{\omega}$, as in Proposition 4.7) if $\omega^{(k-1)} \neq \emptyset$, and $f'(x', x'') = 1$ otherwise. Assume ω_p is connected. Then*

$$f(rx', x'')/rf'(x', x'')$$

extends to a continuous, nowhere vanishing function on $\Sigma(\Omega) = [0, a) \times \Sigma(\omega_p) \times B^l$.

Proof. Assume first that $\omega^{(k-1)} \neq \emptyset$, where $\omega^{(k)}$ is defined as in Proposition 4.7. Let f_0 and f_0' be defined in the same way f and f' were defined, but replacing g with a constant metric g_0. Then the proof of Proposition 4.7 gives that $f_0(rx', x'')/rf_0'(x', x'')$ is independent of r. Hence $f_0(rx', x'')/rf_0'(x', x'')$ extends to a continuous, nowhere vanishing function on $\Sigma(\Omega)$, as it was shown in the proof of Proposition 4.7. Then

$$\frac{f(rx', x'')}{rf'(x', x'')} = \frac{f(rx', x'')}{f_0(rx', x'')} \times \frac{f_0(rx', x'')}{rf_0'(rx', x'')} \times \frac{f_0'(x', x'')}{f'(x', x'')} .$$

We have just argued that the middle quotient in the above product extends to a continuous function on $\Sigma(\Omega)$. The other two quotients also extend to continuous functions on $\Sigma(\Omega)$, by Proposition 4.7 applied to Ω and ω.
Let us assume now that $\omega^{(k-1)} = \emptyset$. Then the same proof applies, given that $f_0'/f' = 1$ clearly extends to a continuous function on $\Sigma(\Omega)$. □

4.3 The weight function r_Ω

Recall that $\eta_{n-2}(x)$, given in Definition 2.5, denotes the distance from $x \in \overline{\Omega}$ to the singular set $\Omega^{(n-2)}$.
The main goal of this subsection is to define on any curvilinear polyhedral domain Ω a function

$$r_\Omega : \overline{\Omega} \to [0, \infty)$$

that lifts to a *smooth* function on $\Sigma(\Omega)$ and is *equivalent* to η_{n-2}. (Additional properties of r_Ω will be established later on.) This will lead to a definition of the Sobolev spaces $\mathcal{K}_a^m(\Omega)$ as weighted Sobolev spaces on Lie manifolds with boundary, Proposition 5.7. We again proceed by induction on n.
We define $r_\Omega = 1$ if $n \leq 1$ (recall $\Omega^{(n-2)} = \emptyset$ if $n < 2$) or if $\Omega^{(n-2)} = \emptyset$, that is, Ω is a smooth manifold, possibly with boundary.
Assume now that a function r_ω was defined for all curvilinear polyhedral domains ω of dimension $< n$ and let us define it for a given bounded n-dimensional curvilinear polyhedral domain Ω.
We localize first to a neighborhood of a generic point $p \in \partial\Omega$ and then use a partition of unity argument. We recall that by definition there exists a

neighborhood V_p of p in M, a diffeomorphism $\phi_p : V_p \to B^{n-l} \times B^l$, for some $0 \leq l = \ell(p) \leq n-1$, and a polyhedral domain $\omega_p \subset S^{n-l-1}$ such that $\phi_p(V_p \cap \Omega) = I\,\omega_p \times B^l$, $I = (0, \epsilon)$, see Condition (18)). Therefore, we can assume that ϕ_p is the identity map and replace in what follows V_p with $\phi_p^{-1}\big(\frac{1}{2}B^{n-l} \times \frac{1}{2}B^l\big)$. Since r_Ω is already defined equal to 1 if $p \in \Omega^{(n-1)} \smallsetminus \Omega^{(n-2)}$, we restrict $n - l - 1 \geq 1$ above. Let r_{ω_p} be the function associated to the curvilinear polyhedral domain ω_p. Then we define

$$r_{V_P}(rx', x'') := r r_{\omega_p}(x'), \quad (rx', x'') \in \Omega \subset V_p, \tag{33}$$

if $x' \in \omega_p$, $x'' \in B^l$, and $1 \leq l = \ell(p) \leq n-2$. Following our usual procedures, we set $r_{V_p}(rx') = r r_{\omega_p}(x')$ if $l = 0$.

We consider next a locally finite covering of $\overline{\Omega}$ with open sets U_α of one of the three following forms

(i) $U_\alpha \subset \overline{U_\alpha} \subset \Omega$ with ∂U_α smooth;

(ii) $U_\alpha = V_p$ with $\ell(p) = n-1$ (*i.e.*, p is not in the singular set of $\overline{\Omega}$); or

(iii) such that for any $x \in U_\alpha \cap \Omega$, the point of $\Omega^{(n-2)}$ closest to x is in V_p with $\ell(p) \leq n-2$, and

$$p \in U_\alpha \subset \overline{U}_\alpha \subset V_p. \tag{34}$$

A condition similar to (iii) above was already used in the proof of Proposition 4.7. The conditions (i) and (ii) above correspond exactly to the case when $(\partial U_\alpha \cap \partial\Omega)$ is smooth (this includes the case when $(\partial U_\alpha \cap \partial\Omega)$ is empty).

We then set

$$r_\alpha = \begin{cases} 1 & \text{if } (\partial U_\alpha \cap \partial\Omega) \text{ is smooth} \\ r_{V_p} & \text{if } U_\alpha \text{ is as in (34).} \end{cases} \tag{35}$$

and define

$$r_\Omega = \sum_\alpha \varphi_\alpha r_\alpha, \tag{36}$$

where φ_α is a smooth partition of unity subordinated to U_α. If Ω is not bounded, we define instead:

$$r_\Omega = \chi\big(\sum_\alpha \varphi_\alpha r_\alpha\big), \tag{37}$$

where χ is defined as in (23). We notice that the definition of r_Ω is not canonical, because it depends on a choice of a covering $\{U_\alpha\}$ of $\overline{\Omega}$ as above and a choice of a subordinated partition of unity.

Proposition 4.9. *Let Ω be a curvilinear, stratified polyhedral domain of dimension $n \geq 2$. Then r_Ω defined in Equation* (36) *(or* (37)*) is continuous on $\overline{\Omega}$ and $r_\Omega \circ \kappa$ is smooth on $\Sigma(\Omega)$. Moreover, η_{n-2}/r_Ω extends to a continuous, nowhere vanishing function on $\Sigma(\Omega)$ and r_α/r_Ω extends to a smooth function on $\Sigma(V_p \cap \Omega)$.*

Proof. Let $\eta_{-1} := 1$ for the inductive step. We shall prove the statement on η_{n-2}/r_Ω by induction on $n \geq 1$. Since $r_\Omega = 1$ for polyhedral domains of dimension $n = 0$, the result is obviously true for $n = 1$. We now proceed with the inductive step.

We shall use the above results, in particular, Proposition 4.7, for $k = n-2 \geq 0$. Thus $f = \eta_{n-2}$ in the notation of Proposition 4.7. Let $f_\alpha(x)$ be the distance from $x \in V_p$ to $V_p \cap \Omega^{(n-2)}$, if $U_\alpha \subset V_p$ is as in Equation (34) (so $\ell(p) \leq n-2$ in this case). Thus $f_\alpha = f$ on $U_\alpha \cap \Omega$, by the construction of U_α. We identify once again $V_p \cap \Omega$ with $(0,\epsilon)\,\omega_p \times B^l$, $l = \ell(p)$, using the diffeomorphism ϕ_p, and set again $\omega := \omega_p \times B^l$. Also, for any $x \in \omega$, let $f'_\alpha(x)$ be the distance from x to the singular set $\omega^{(n-l-2)}$ of ω if it is not empty, $f'_\alpha(x) = 1$ otherwise. Let r_α be as in the definition of r_Ω, Equation (36). Then

$$\frac{f_\alpha(rx', x'')}{r_\alpha(rx', x'')} = \frac{f_\alpha(rx', x'')}{rf'_\alpha(x', x'')}\,\frac{f'_\alpha(x', x'')}{r_{\omega_p}(x', x'')}\,, \qquad \text{for } (rx', x'') \in V_p \cap \Omega.$$

The quotient $f'_\alpha(rx', x'')/rf'_\alpha(x', x'')$ extends to a continuous, nowhere vanishing function on $\Sigma(V_p \cap \Omega)$, by Corollary 4.8. By the induction hypothesis, the quotient $f'_\alpha(x', x'')/r_{\omega_p}(x', x'')$ also extends to a continuous, nowhere vanishing function on $\Sigma(\omega) = \Sigma(\omega_p) \times B^l$. Since this quotient is independent of r, it also extends to a continuous, nowhere vanishing function on $\Sigma(V_p \cap \Omega)$. Hence f_α/r_α extends to a continuous, nowhere vanishing function on $\Sigma(V_p)$. Therefore

$$r/f = \sum_\alpha \varphi_\alpha r_\alpha/f = \sum_\alpha \varphi_\alpha r_\alpha/f_\alpha$$

extends to a continuous function on $\Sigma(\Omega)$.

The quotient r/f is immediately seen to be non-zero everywhere, from the definition. Hence f/r also extends to a continuous function on $\Sigma(\Omega)$.

We have already noticed that r_α/f extends to a continuous, nowhere vanishing function on $\Sigma(V_p)$. Hence $r_\alpha/r_\Omega = (r_\alpha/f)(f/r_\Omega)$ extends to a continuous, nowhere vanishing function on $\Sigma(V_p \cap \Omega)$. Since both r_α and r_Ω are smooth on $\Sigma(V_p \cap \Omega)$ and the set of zeroes of r_Ω is the union of transversal manifolds on which r_Ω has simple zeroes, it follows that r_α/r_Ω extends to a smooth function on $\Sigma(V_p)$. Since $\overline{U}_\alpha \subset V_p$ is compact, it follows from a compactness argument that r_α and r are equivalent on U_α. The proof is complete. ☐

We can now prove the following result, which will be used in the proof of Theorem 6.4.

Proposition 4.10. *Let Ω be a bounded, curvilinear, stratified polyhedral domain. Suppose r_Ω, r'_Ω are two functions on $\overline{\Omega}$ defined by formula* (36) *(or* (37)*) with possibly different choices of open covering $\{U_\alpha\}$, subordinate partition $\{\varphi_\alpha\}$, and diffeomorphisms ϕ_p. Then r'_Ω/r_Ω extends to a smooth, nowhere vanishing function on $\Sigma(\Omega)$.*

Proof. We know from Proposition 4.9, that f/r'_Ω and f/r_Ω extend to continuous, nowhere vanishing functions on $\Sigma(\Omega)$. Hence r'_Ω/r_Ω extends to a continuous, nowhere vanishing function on $\Sigma(\Omega)$. Since both r'_Ω and r_Ω are smooth functions on $\Sigma(\Omega)$ and the set of zeroes of r_Ω is a union of transverse manifolds, each a set of simple zeroes of r_Ω, it follows that the quotient r'_Ω/r_Ω is smooth on $\Sigma(\Omega)$. □

We obtain the following corollary. Let $H \subset \Sigma(\Omega)$ be a hyperface (*i.e.,* face of maximal dimension) of $\Sigma(\Omega)$. Recall that *a defining function of H* is a smooth function $x_H \geq 0$ defined on $\Sigma(\Omega)$, such that $H = \{x = 0\}$ and $dx_H \neq 0$ on H. All the faces of $\Sigma(\Omega)$ are closed subsets of $\Sigma(\Omega)$, by definition. We have already noticed that any face of $\Sigma(\Omega)$ has a defining function. We then have the following corollary.

Corollary 4.11. *Let $\eta = \prod_H x_H$, where H ranges through the set of hyperfaces of $\Sigma(\Omega)$ that do not intersect $\partial\Omega \smallsetminus \Omega^{(n-2)}$. Then η/r_Ω extends to a smooth, nowhere vanishing function on $\Sigma(\Omega)$.*

Proof. This is a local statement that can be checked by induction, as in the previous proofs. □

In particular, since the function r_Ω is anyway determined only up to a factor of $h \in \mathcal{C}^\infty(\Sigma(\Omega))$, $h \neq 0$, we obtain that we could take $r_\Omega = \prod_H x_H$, where H ranges through the set of hyperfaces of $\Sigma(\Omega)$ that do not intersect $\partial\Omega \smallsetminus \Omega^{(n-2)}$. The function r_Ω, for various versions of the set Ω, will play an important role in the inductive definition of the structural Lie algebra of vector fields $\mathcal{V}(\Omega)$ on $\Sigma(\Omega)$, which we address next. The faces considered in the above corollary are the hyperfaces at infinity of $\Sigma(\Omega)$. See Definition 3.8.

4.4 The structural Lie algebra of vector fields

We now proceed to define by induction a canonical Lie algebra of vector fields $\mathcal{V}(\Omega)$ on $\Sigma(\Omega)$, for Ω a curvilinear, stratified polyhedral domain of dimension $n \geq 1$. In view of Corollary 4.3, we can assume that Ω is connected. We denote by

$$\mathcal{X}(M) := \Gamma\big(M; TM\big)$$

the space of vector fields on a manifold M. We let

$$\mathcal{V}(\Omega) = \mathcal{X}(\overline{\Omega}) = \mathcal{X}(\Sigma(\Omega)), \quad \text{if } n = 1. \tag{38}$$

In other words, there is no restriction on the vector fields $X \in \mathcal{V}(\Omega)$, if Ω has dimension one.

Assume now that the Lie algebra of vector fields $\mathcal{V}(\omega)$ has been defined on $\Sigma(\omega)$ for all curvilinear polyhedral domains ω of dimension $1 \leq k \leq n-1$ and let us define $\mathcal{V}(\Omega)$ for a curvilinear polyhedral domain of dimension n. We fix $p \in \partial\Omega$ and let V_p and ϕ_p be as in Definition 2.1, as usual. We identify $V_p \cap \Omega$ with $(0,1)\omega_p \times B^l$ using ϕ_p. Assume $1 \leq \ell(p) \leq n-2$, so that in particular ω_p is a curvilinear polyhedral domain of dimension ≥ 1. Let $M_1 := [0,1) \times \Sigma(\omega_p) \times B^l$. We notice that

$$TM_1 = T([0,1) \times \Sigma(\omega_p) \times B^l) = T([0,1)) \times T\Sigma(\omega_p) \times TB^l$$

and hence

$$\begin{aligned}\mathcal{X}\big(M_1\big) = \Gamma\big(M_1;\, T[0,1)\big) \times_{M_1} \Gamma\big(M_1;\, T\Sigma(\omega_p)\big) \times_{M_1} \Gamma\big(M_1;\, TB^l\big)\\ \subset \Gamma\big(M_1;\, T[0,1)\big) \times \Gamma\big(M_1;\, T\Sigma(\omega_p)\big) \times \Gamma\big(M_1;\, TB^l\big).\end{aligned}$$

Then we define

$$\begin{aligned}\mathcal{V}(V_p \cap \Omega) = \{X = (X_1, X_2, X_3) \in \mathcal{X}\big(M_1\big)\\ X_1 \in \Gamma\big(M_1;\, T[0,1)\big), \quad X_2 \in \Gamma\big(M_1;\, T\Sigma(\omega_p)\big), \quad X_3 \in \Gamma\big(M_1;\, TB^l\big)\\ Y_1 := r_\Omega^{-1} X_1 \text{ and } Y_3 := r_\Omega^{-1} X_3 \text{ are smooth, and}\\ X_2(t, x', x'') \in \mathcal{V}\big(\{t\} \times \omega_p \times \{x''\}\big) = \mathcal{V}(\omega_p), \quad \text{for any fixed } t, x''\}. \quad (39)\end{aligned}$$

In Equation (39) above, "smooth" means, "smooth *including at* $r = 0$." If $\ell(p) = 0$, then we just drop the component X_3, but keep the same conditions on X_1 and X_2. By Proposition 4.10, the definition of $\mathcal{V}(V_p \cap \Omega)$ is independent of the choice of r_Ω. All vector fields are assumed to be smooth.
Finally, we define $\mathcal{V}(\Omega)$ to consist of the vector fields $X \in \mathcal{X}(\Sigma(\Omega))$ such that $X|_{V_p \cap \Omega} \in \mathcal{V}(V_p \cap \Omega)$ for all $p \in \Omega^{(n-2)}$. In particular, only the smoothness condition is imposed on our vector fields at the smooth points of $\partial\Omega$. Note that the vector fields in $\mathcal{V}(\Omega)$ may not extend to the closure $\overline{\Omega}$, in general. This was seen in Example 2.10.

4.5 Lie manifolds with boundary

We now proceed to show that the pair $(\Sigma(\Omega), \mathcal{V}(\Omega))$ defines a Lie manifold with boundary, introduced in [1], and the construction of which was recalled in Definition 3.5.
We first establish some lemmata.

Lemma 4.12. *Let $X \in \mathcal{X}(\Sigma(\Omega))$ be such that $X = 0$ in a neighborhood of the boundary of $\Sigma(\Omega)$. Then $X \in \mathcal{V}(\Omega)$.*

Proof. The result follows immediately by induction from the definition of $\mathcal{V}(\Omega)$. □

We also get the following simple fact.

Lemma 4.13. *If $f : \Sigma(\Omega) \to \mathbb{C}$ is a smooth function and $X \in \mathcal{V}(\Omega)$, then $X(f)$ is a smooth function on $\Sigma(\Omega)$ and $fX \in \mathcal{V}$.*

Proof. The vector field X is smooth on $\Sigma(\Omega)$, hence $X(f)$ is smooth on $\Sigma(\Omega)$. The second statement is local, so it is enough to check it on Ω and on each V_p, on which it is as a direct consequence of the definition and induction. □

Lemma 4.14. *For any $X \in \mathcal{V}(\Omega)$ and any continuous function $f : \overline{\Omega} \to \mathbb{C}$ such that $f \circ \kappa$ is smooth on $\Sigma(\Omega)$, we have*

$$X(f) = \tilde{f}\, r_\Omega,$$

where $\tilde{f}$ is a smooth function on $\Sigma(\Omega)$. In particular, $X(r_\Omega) = f_X r_\Omega$, where f_X is a smooth function on $\Sigma(\Omega)$.

Proof. This is a local statement that can be checked by induction in any neighborhood V_p, using the definition, as follows. Let us use the notation of Equation (39) and write

$$X = (X_1, 0, 0) + (0, X_2, 0) + (0, 0, X_3).$$

We shall write, with abuse of notation, $X_1 = (X_1, 0, 0)$. Define X_2 and X_3 similarly. It is enough to check that $X_j f(rx', x'')$ is of the indicated form, for $j = 1, 2, 3$. We have $X_1 = r_\Omega Y_1$ and $X_3 = r_\Omega Y_3$, where Y_1 and Y_3 are smooth (in appropriate spaces), by Equation (39). This observation proves our lemma if $X = X_1$ or $X = X_3$. If $X = X_2$, then we have

$$(Xf)(r, x', x'') = X_2(f(rx', x'')) = r_{\omega_p} f_1(r, x', x''), \tag{40}$$

with f_1 a smooth function on $\Sigma(V_p \cap \Omega) = [0, \epsilon) \times \Sigma(\omega_p) \times \mathbb{R}^l$, by the induction hypothesis. Moreover, given that by assumption (39) $\kappa_* X$ is a vector field tangent to the sphere S^{n-l-1}, we see that $Xf(0, x', x'') = 0$. Therefore $Xf = r r_{\omega_p} \tilde{f}$, for some smooth function $\tilde{f}$ on $\Sigma(V_p \cap \Omega)$. Let us denote $r_\alpha = r r_{\omega_p}$, as in Equation (35) and in Proposition 4.9. Proposition 4.9 gives that r_α / r_Ω is smooth on its domain of definition. Hence $Xf = r_\alpha f_1 = r_\Omega (r_\alpha / r_\Omega) f_1 = r_\Omega \tilde{f}$, with $\tilde{f}$ smooth on each $\Sigma(V_p \cap \Omega)$. Hence $\tilde{f}$ is smooth on $\Sigma(\Omega)$. □

We next characterize which vector fields on Ω are restrictions of vector fields on $\mathcal{V}(\Omega)$. We begin by showing that the restriction property is local.

Lemma 4.15. *Let Y be a vector field on Ω with the property that every point $p \in \overline{\Omega}$ has a neighborhood U_p in M such that $Y = X_U$ on $U \cap \Omega$, for some $X_U \in \mathcal{V}(\Omega)$. Then there exists $X \in \mathcal{V}(\Omega)$ such that Y is the restriction of X to Ω.*

Proof. Let us cover $\overline{\Omega}$ with a locally finite family of sets U_p, $p \in B \subset \overline{\Omega}$. Let ψ_p, $p \in B$, be a subordinated partition of unity.
We claim that $X = \sum_{p \in B} \psi_p X_{U_p} \in \mathcal{V}(\Omega)$ (by Lemma 4.13) satisfies $X(x) = Y(x)$, $x \in \Omega$. Indeed, $X(x) = \sum_{p \in B} \psi_p(x) X_{U_p}(x) = \big(\sum \psi_p(x)\big) Y(x) = Y(x)$. □

We can now prove the following lemma.

Lemma 4.16. *Let Y be a smooth vector field on $\overline{\Omega}$. Then $r_\Omega Y$ is the restriction to $\Omega \subset \Sigma(\Omega)$ of a vector field X in $\mathcal{V}(\Omega)$.*

Proof. By Lemma 4.15, it is enough to check this statement on a neighborhood V_p of some $p \in \partial\Omega$. We shall proceed by induction. Since the desingularization and the definition of r_Ω are covariant with respect to diffeomorphism (that respect the stratification of Ω), we can assume that $V_p = B^{n-l} \times B^l$ and that $V_p \cap \Omega \simeq (0,1)\omega_p \times B^l$. Assume first that $Y = \partial_j$ is a constant vector field on V_p. Let $\alpha_t(x', x'') = (tx', x'')$. Then $D\alpha_t(\partial_j) = t\partial_j$. Therefore,

$$D\alpha_t(X) = X, \tag{41}$$

where $X = r_\Omega \partial_j$, where r_Ω can be taken, on V_p, to be given by rr_{ω_p}. Let us decompose $\partial_j = (Y_1, Y_2, Y_3)$ on V_p using the notation of Equation (39). Then Y_3 is constant. In fact, either $Y_3 = \partial_j$ or $Y_3 = 0$. In any instance, if we write $X = (X_1, X_2, X_3)$, then $X_3 = r_\Omega Y_3$ satisfies the condition of Equation (39). The relation (41) gives that $Y_1(r, x', x'') = a_1(x')\partial_r$ and $Y_2(r, x', x'') = r^{-1}Z(x')$, with a_1 a smooth function and Z a smooth vector field on $\overline{\omega}_p$. Clearly $X_1 = r_\Omega Y_1$ will satisfy the conditions of Equation (39). The induction hypothesis then gives that $X_2(r, x', x'') = r_\Omega Y_2(r, x', x'') = r_{\omega_p}(x')Z(x')$ is the restriction to $V_p \cap \Omega$ of a smooth vector field in $\mathcal{V}(V_p \cap \Omega)$. (This vector field depends only on the second factor in $\Sigma(V_p \cap \Omega) = [0,1) \times \omega_p \times B^l$.) □

We now identify a canonical metric on the vector fields $\mathcal{V}$. Recall that the concept of local basis of a space of vector fields was defined in Definition 3.1.

Proposition 4.17. *Let us fix a metric h on $M \supset \Omega$. Let $q \in \Sigma(\Omega)$ be arbitrary. Then there exists a neighborhood U of q in $\Sigma(\Omega)$ and $X_1, X_2, \ldots, X_n \in \mathcal{V}(\Omega)$ that form a local basis of $\mathcal{V}(\Omega)$ on U and satisfy*

$$h(X_j, X_k) = r_\Omega^2 \delta_{jk}.$$

In other words, the vectors $X_1, X_2, \ldots, X_n$ form an orthonormal system on $\Omega \cap U$ for the metric $r_\Omega^{-2}h$. A local basis $X_1, X_2, \ldots, X_n$ with this property will be called *a local orthonormal basis of $\mathcal{V}(\Omega)$ over U.*

Proof. If $q \in \Omega \subset \Sigma(\Omega)$, the result follows from Lemma 4.12. Let $p = \kappa(q)$. We shall hence assume that $p \in \partial\Omega$. This is again a local statement in $p \in \partial\Omega$. We can therefore proceed by induction. If the dimension n of Ω is 1, then there is nothing to prove because $r_\Omega = 1$ in this case.
Once again, we let $\phi_p : V_p \to B^{n-l} \times B^l$ and ω_p be as in Definition 2.1. We can assume that ϕ_p is the identity map. If we can prove the result for the function $r = r_\Omega$, then we can prove it for the function $r' = f'r$, where $f', 1/f' \in \mathcal{C}^\infty(\Sigma(\Omega))$, simply by replacing X_j with $f'X_j$. By Proposition 4.9, we can therefore assume that $r_\Omega = rr_{\omega_p}$ on $V_p \cap \Omega$. Let $q = (0, x', x'') \in [0,1) \times \Sigma(\omega_p) \times B^l$.
Let h_0 be the standard metric on V_p. For the induction hypothesis, we shall need that the metric h_0 is given by

$$h_0(r, x', x'') = (dr)^2 + r^2(dx')^2 + (dx'')^2 \tag{42}$$

on $\Omega \cap V_p = (0,1)\omega_p \times B^l$. Here $(dx')^2$ denotes the metric on ω_p induced by the Euclidean metric on the sphere S^{n-l-1}. In other words, if $X = (X_1, X_2, X_3)$ is a vector field on $V_p \cap \Omega$, written using the product decomposition explained above (or as in the Equation (39)), then

$$h_0(X) = \|X_1\|^2 + r^2\|X_2\|^2 + \|X_3\|^2$$

where the norms come from the standard metrics, respectively, on $T[0,1)$, on $TS^{n-l-1} \supset T\omega_p$, and on $T\mathbb{R}^l$.
Let us assume first that $h = h_0$, the standard metric on $\mathbb{R}^n$. By the induction hypothesis, we can construct $Y_2, \ldots, Y_{n-l} \in \mathcal{V}(\omega_p)$ forming a local orthonormal basis of $\mathcal{V}$ over some small neighborhood U' of x' in $\Sigma(\omega_p)$ (*i.e.,* $\{Y_2, \ldots, Y_{n-l}\} \subset \mathcal{V}(\omega_p)$ is orthonormal with respect to the metric $r_{\omega_p}^{-2}(dx')^2$). Here $(dx')^2$ denotes the metric on ω_p induced by the Euclidean metric on the sphere S^{n-l-1}, as above. Let $Y_1 = r_\Omega \partial_r$ and $Y_j = r_\Omega \partial_j$, $j = n-l+1, \ldots, n$, where ∂_j forms the standard basis of $\mathbb{R}^{l-1}$. Then we claim that we can take $U = [0,1) \times U' \times B^l$ and

$$\{X_1, X_2, \ldots, X_n\} = \{Y_1\} \cup \{Y_2, \ldots, Y_{n-l}\} \cup \{Y_{n-l+1}, \ldots, Y_n\}. \tag{43}$$

(If $n-l = 1$, then the second set in the above union is empty. If $l = 0$, then the third set in the above union is empty.) Indeed, $\{X_1, \ldots, X_n\}$ is a local basis by construction and by the local definition of $\mathcal{V}(\Omega)$ in Equation (39). Let us check that this is an orthonormal local basis. To this end, we shall use the form of the standard metric h_0 given in Equation (42), to obtain

$$h_0(X_1) = r_\Omega^2 \|\partial_r\|^2 = r_\Omega^2\,, \quad h_0(X_{n-l+1}) = \ldots = h_0(X_n) = r_\Omega^2$$
$$\text{and } \ h_0(X_2) = \ldots = h_0(X_{n-l}) = r^2\|X_2\|^2 = r^2 r_{\omega_p}^2 = r_\Omega^2\,.$$

It is also clear that $\{X_1, X_2, \ldots, X_n\}$ is an orthogonal system. This completes the induction step if $h = h_0$, the standard metric on $\mathbb{R}^n$.
If h is not the standard metric on V_l, we can nevertheless chose a matrix valued function T defined on a neighborhood of q in U such that $h(T\xi, T\eta) = h_0(\xi, \eta)$. We then let $X_j = TY_j$ and replace U with this smaller neighborhood. $\square$

This lemma gives the following corollary.

Corollary 4.18. *Let $X, Y \in \mathcal{V}(\Omega)$ and h be a fixed metric on M. Then the function $r_\Omega^{-2}h(X,Y)$, defined first on Ω, extends to a smooth function on $\Sigma(\Omega)$.*

Proof. This is a local statement in the neighborhood of each point $q \in \Sigma(\Omega)$. Let $X_1, X_2, \ldots, X_n$ be a local basis of $\mathcal{V}$ on a neighborhood U of q in $\Sigma(\Omega)$ satisfying the conditions of Proposition 4.17 (*i.e.,* orthogonal with respect to $r_\Omega^{-2}h$). Let $X = \sum \phi_j X_j$ and $Y = \sum \psi_j X_j$ on $U \cap \Omega$, where ϕ_j, ψ_j are smooth functions on $\Sigma(\Omega)$. Then $r_\Omega^{-2}h(X,Y) = \sum \phi_j \overline{\psi}_j$ is smooth on U. $\square$

Lemma 4.19. *Let $p \in \partial\Omega$ and $X_1, X_2, \dots, X_n$ be vector fields on $\overline{\Omega}$ that define a local basis of TM on $\overline{U}$, for some neighborhood U of p. Then $r_\Omega X_1, r_\Omega X_2, \dots, r_\Omega X_n$ is a local basis of $\mathcal{V}(\Omega)$ on U, that is, for any $Y \in \mathcal{V}(\Omega)$, there exist unique smooth function $\phi_1, \phi_2, \dots, \phi_n$ on $\Sigma(\Omega)$ satisfying*

$$Y = \phi_1 r_\Omega X_1 + \phi_2 r_\Omega X_2 + \ldots + \phi_n r_\Omega X_n \quad \text{on } U \cap \Omega \subset \Sigma(\Omega). \tag{44}$$

Conversely, if a vector field Y on Ω satisfies Condition (44) for any p and any local basis $X_1, \dots, X_n$ of TM at p, then Y is the restriction to Ω of a vector field in $\mathcal{V}(\Omega)$.

Proof. The converse part is easier, so we prove it first. Let Y be a vector field on Ω that satisfies Condition (44) for any p and any local basis $X_1, \dots, X_n$ of TM at p. Fix an arbitrary $p \in \Omega$. Lemmata 4.13 and 4.16 give that $\phi_j r_\Omega X_j$ is the restriction to Ω of a vector field in $\mathcal{V}(\Omega)$. Hence on each $U \cap \Omega$, Y is the restriction of a vector field $Y_U \in \mathcal{V}(\Omega)$. Lemma 4.15 then gives the converse part of our lemma.

We now prove the direct part of the lemma. We can assume that the vector fields $X_1, \dots, X_n$ form an orthonormal system on U with respect to some fixed metric h on M. We know from Lemma 4.16 that $r_\Omega X_j \in \mathcal{V}(\Omega)$.

Let then $Y \in \mathcal{V}(\Omega)$ and note that $\phi_j = r_\Omega^{-1} h(Y, X_j) = r_\Omega^{-2} h(Y, r_\Omega X_j) \in \mathcal{C}^\infty(\Sigma(\Omega))$, by Corollary 4.18. Then $Y = \sum_{j=1}^n \phi_j r_\Omega X_j$ on $U \cap \Omega$. The local uniqueness of the functions ϕ_j follows from the fact that $r_\Omega X_1, r_\Omega X_2, \dots, r_\Omega X_n$ also form a local basis of $T\Omega$ on $U \cap \Omega$. □

We are now ready to prove the following characterizations of $\mathcal{V}(\Omega)$. We notice that the restriction map $\mathcal{V}(\Omega) \ni X \to X|_\Omega$ is injective, so we may identify $\mathcal{V}(\Omega)$ with a subspace of the space $\Gamma(\Omega, TM)$ of vector fields on Ω.

Proposition 4.20. *Let $\Omega \subset M$ be a curvilinear, stratified polyhedral domain of dimension n and let X be a smooth vector field on Ω. Fix an arbitrary metric h on M. Then $X \in \mathcal{V}(\Omega)$ if, and only if, $r_\Omega^{-1} h(X, Y)$ extends to a smooth function on $\Sigma(\Omega)$ for any smooth vector field Y on $\overline{\Omega}$.*

Proof. In one direction the result follows from Lemma 4.16 and Corollary 4.18. Indeed, let $X \in \mathcal{V}(\Omega)$ and Y be a smooth vector field on $\overline{\Omega}$. Then $r_\Omega Y \in \mathcal{V}(\Omega)$ by Lemma 4.16 and hence $r_\Omega^{-1} h(X, Y) = r_\Omega^{-2} h(X, r_\Omega Y)$ extends to a smooth function on $\Sigma(\Omega)$ by Corollary 4.18. (We have already used this argument in the proof of the previous lemma.)

Conversely, assume that $r_\Omega^{-1} h(X, Y)$ extends to a smooth function on $\Sigma(\Omega)$ for any smooth vector field on $\overline{\Omega}$. The statement that $X \in \mathcal{V}(\Omega)$ is a local statement, by Lemma 4.15. So let $p \in \overline{\Omega}$ and let U be an arbitrary neighborhood of p. Choose smooth vector fields defined in a neighborhood of $\overline{\Omega}$ in M such that $X_1, X_2, \dots, X_n$ is a local orthonormal basis on U (orthonormal with respect to h). Let

$$\phi_j = r_\Omega^{-1} h(Y, X_j),$$

by assumption $\phi_j \in \mathcal{C}^\infty(\Sigma(\Omega))$. Then $Y = \sum_{j=1}^n \phi_j X_j$ on $U \cap \Omega$ and $\sum_{j=1}^n \phi_j X_j \in \mathcal{V}(\Omega)$. Lemma 4.15 then shows that $X \in \mathcal{V}(\Omega)$. □

We now prove the main characterization of the structural Lie algebra of vector fields $\mathcal{V}(\Omega)$.

Theorem 4.21. *Let $\Omega \subset M$ be a bounded curvilinear, stratified polyhedral domain of dimension n. Then $\mathcal{V}(\Omega)$ is generated as a vector space by the vector fields of the form $\phi\, r_\Omega X$, where $\phi \in \mathcal{C}^\infty(\Sigma(\Omega))$ and X is a smooth vector field on $\overline{\Omega}$.*

Proof. We know that $\phi r_\Omega X \in \mathcal{V}(\Omega)$ whenever X is a smooth vector field on $\overline{\Omega}$, by Lemmata 4.13 and 4.16. This remark shows that the linear span of vectors of the form $\phi\, r_\Omega X$, where $\phi \in \mathcal{C}^\infty(\Sigma(\Omega))$ and X is a smooth vector field in a neighborhood of Σ, is contained in $\mathcal{V}(\Omega)$.
Conversely, let $Y \in \mathcal{V}(\Omega)$. Then Lemma 4.19 shows that we can find, in the neighborhood U_p of any point $p \in \overline{\Omega}$ vector fields $X_{1p}, X_{2p}, \ldots, X_{np}$ and smooth functions ϕ_{jp} such that $Y = \sum \phi_{jp} r_\Omega X_{jp}$ on U_p. The result then follows using a finite partition of unity on $\Sigma(\Omega)$ subordinated to the covering U_p. □

If we drop the condition that Ω be bounded, we obtain the following result, which was established in the first half of the above proof.

Proposition 4.22. *Let $\Omega \subset M$ be a curvilinear polyhedral domain of dimension n. Then $\mathcal{V}(\Omega)$ consists of the set of vector fields that locally can be written as linear combinations of vector fields of the form $\phi r_\Omega X$, where $\phi \in \mathcal{C}^\infty(\Sigma(\Omega))$ and X is a smooth vector field on $\overline{\Omega}$.*

We are finally in the position to endow $\Sigma(\Omega)$ with a structure of Lie manifold, which we will exploit in the following sections to study the mixed boundary value/interface problem (6). We set $\partial''\Sigma(\Omega)$ to be the union of all hyperfaces (*i.e.,* faces of maximal dimension) H of $\Sigma(\Omega)$ such that $\kappa(H) \subset \overline{\Omega}$ lies in the singular set $\Omega^{(n-2)}$, and let $\partial'\Sigma(\Omega) = \partial\Sigma(\Omega) \smallsetminus \partial''\Sigma(\Omega)$. In particular, $\partial''\Sigma(\Omega)$ is the union of the hyperfaces at infinity of $\Sigma(\Omega)$, see Definition 3.8. The next theorem is the main result of this subsection.

Theorem 4.23. *Let Ω be a bounded curvilinear, stratified polyhedral domain and let*

$$\mathfrak{D}_0 := \Sigma(\Omega) \smallsetminus \partial''\Sigma(\Omega) = \Omega \cup \partial'\Sigma(\Omega) = \kappa^{-1}(\overline{\Omega} \smallsetminus \Omega^{(n-2)}).$$

Then $(\mathfrak{D}_0, \Sigma(\Omega), \mathcal{V}(\Omega))$ is a Lie manifold with boundary $\partial'\Sigma(\Omega)$. The projection map $\kappa : \mathfrak{D}_0 \to \overline{\Omega} \smallsetminus \Omega^{(n-2)}$ is such that $\kappa^{-1}(p)$ consists of exactly one point if $p \in \overline{\Omega} \smallsetminus \Omega^{(n-2)}$.

Proof. The last statement (on the number of elements in $\kappa^{-1}(p)$, $p \in \overline{\Omega} \smallsetminus \Omega^{(n-2)}$) follows from the definition. Therefore, to prove the proposition, we need, using the notation of Definition 3.5, to construct a compactification $\mathfrak{D}$ of $\mathfrak{D}_0$ that identifies with the closure of a Lie domain in a Lie manifold $\mathfrak{M}$.
We shall choose then $\mathfrak{D} = \Sigma(\Omega)$. Then we shall let $\mathfrak{M}$ be the "double" of $\Sigma(\Omega)$, also denoted ${}^d\Sigma(\Omega)$. More precisely, $\mathfrak{M}$ is obtained from the disjoint union of

two copies of $\Sigma(\Omega)$ by identifying the hyperfaces that are not at infinity. We let $\mathcal{V}$ to be the set of smooth vector fields on $\mathfrak{M}$ such that the restriction to either copy of $\Sigma(\Omega)$ is in $\mathcal{V}(\Omega)$.

Let $\mathbb{D}$ be obtained from the closure of Ω in $\mathfrak{M}$ by removing the closure of $\partial'\Sigma(\Omega)$. Then $\mathbb{D}$ is an open subset of $\mathfrak{M}$ whose closure is $\Sigma(\Omega)$. Moreover, $\partial_{\mathfrak{M}}\mathbb{D}$ (the boundary of $\mathbb{D}$ regarded as a subset of $\mathfrak{M}$) is the closure of $\partial'\Sigma(\Omega)$. To prove our theorem, we shall check that $\mathfrak{M}$ is a manifold with corners, that $(\mathfrak{M}, \mathcal{V})$ is a Lie manifold, and that $\partial\mathbb{D}$ is a regular submanifold of $\mathfrak{M}$. Each of these properties is local, so it can be checked in the neighborhood of a point of $\mathfrak{M}$.

Fix $V_p = (0, \epsilon) \times \omega_p \times B^l$. Then the union of the two copies of $\Sigma(V_p)$ is the double ${}^d\Sigma(V_p)$ of $\Sigma(V_p)$. Denote by ${}^d\omega_p$ the double of ω_p. Then

$$ {}^d\Sigma(V_p) = [0, \epsilon) \times {}^d\omega_p \times B^l. $$

An inductive argument then shows that ${}^d\Sigma(\Omega)$ is a manifold with corners and that $\partial\mathbb{D}$ is a regular submanifold of $\mathfrak{M}$.

Let us check that $\mathcal{V}$ satisfies the conditions defining a Lie manifold structure on $\mathfrak{M}$. It follows from Theorem 4.21 that $\mathcal{V}$ is a $\mathcal{C}^\infty(\mathfrak{M})$–module (this checks condition (iii) of Definition 3.2). Theorem 4.21 and Lemmata 4.14, 4.13 show that $\mathcal{V}$ is closed under Lie brackets (this checks condition (i) of Definition 3.2). Condition (ii) of that definition follows from the definition of $\mathcal{V}(\Omega)$. Condition (iv) of Definition 3.2 as well as Condition (ii) of Definition 3.3 were proved in Lemma 4.19. This shows that $(\mathfrak{M}, \mathcal{V})$ is a Lie manifold. □

An immediate consequence of the above Proposition is that the boundary $\partial\mathfrak{D}_0 = \partial'\Sigma(\Omega)$ of $\mathfrak{D}_0 = \Sigma(\Omega) \smallsetminus \partial''\Sigma(\Omega)$ will acquire the structure of a Lie manifold, as explained after the definition of a Lie manifold with boundary, Definition 3.5. Let D be the closure of $\partial\mathfrak{D}_0$ in $\mathfrak{D}$. Then the Lie structure at infinity is $(\partial\mathfrak{D}_0, D, \mathcal{W})$, where

$$ \mathcal{W} = \{X|_D,\, X \in \mathcal{V}, X|_D \text{ is tangent to } D\}. \tag{45} $$

As always, $X \in \mathcal{W}$ is completely determined by its restriction to $\mathfrak{D}_0$.

5 Weighted Sobolev spaces

One of the main goals of this work, as mentioned already, is the study of mixed boundary value/interface problems for second-order elliptic operators on n-dimensional curvilinear, stratified polyhedral domains Ω in the framework of certain weighted Sobolev spaces. This framework is adapted to the singular geometry of polyhedral domains and allows to obtain optimal regularity, which does not hold in general in the standard (unweighted) spaces.

We begin by giving a rigorous definition of the weighted spaces. Let f be a continuous function on Ω, $f > 0$ on the interior of Ω. We define the μ-th

Sobolev space with weight f and index a by

$$\mathcal{K}^{\mu}_{a,f}(\Omega) = \{u \in L^2_{\mathrm{loc}}(\Omega),\ f^{|\alpha|-a}\partial^\alpha u \in L^2(\Omega),\ \text{for all } |\alpha| \leq \mu\}, \quad \mu \in \mathbb{Z}_+. \tag{46}$$

The norm on $\mathcal{K}^{\mu}_{a,f}(\Omega)$ is given by

$$\|u\|^2_{\mathcal{K}^{\mu}_{a,f}(\Omega)} := \sum_{|\alpha|\leq\mu} \|f^{|\alpha|-a}\partial^\alpha u\|^2_{L^2(\Omega)}. \tag{47}$$

Definition 5.1. Let f, g be two continuous, non-negative functions on Ω. We shall say that f and g are *equivalent* (written $f \sim g$) if there exists a constant $C > 0$ such that

$$C^{-1}f(x) \leq g(x) \leq Cf(x),$$

for all $x \in \Omega$.

Clearly, if $f \sim g$, then the norms $\|u\|_{\mathcal{K}^{\mu}_{a,f}(\Omega)}$ and $\|u\|_{\mathcal{K}^{\mu}_{a,g}(\Omega)}$ are equivalent, and hence we have $\mathcal{K}^{\mu}_{a,f}(\Omega) = \mathcal{K}^{\mu}_{a,g}(\Omega)$ as Banach spaces.

Definition 5.2. Let $f = \eta_{n-2}$ be the distance to $\Omega^{(n-2)}$, as before. Then we define $\mathcal{K}^{\mu}_{a}(\Omega) = \mathcal{K}^{\mu}_{a,f}(\Omega)$ and $\|u\|_{\mathcal{K}^{\mu}_{a}(\Omega)} = \|u\|_{\mathcal{K}^{\mu}_{a,f}(\Omega)}$.

For example, $\mathcal{K}^{0}_{0}(\Omega) = L^2(\Omega)$. For Ω a polygon in the plane, $\eta_{n-2}(x) = \eta_0(x)$ is the distance from x to the vertices of Ω and the resulting spaces $\mathcal{K}^{\mu}_{a}(\Omega)$ are the spaces considered in Kondratiev's paper [41]. Above in Definition 5.2, we can and will replace η_{n-2} with the equivalent function r_Ω by Proposition 4.9. If $\mu \in \mathbb{N} = \mathbb{Z}_+ \smallsetminus \{0\}$, we define $\mathcal{K}^{-\mu}_{-a}(\Omega)$ to be the dual of

$$\overset{\circ}{\mathcal{K}^{\mu}_{a}}(\Omega) := \mathcal{K}^{\mu}_{a}(\Omega) \cap \{\partial^j_\nu u|_{\partial\Omega} = 0,\ j = 0, 1, \ldots, \mu - 1\} \tag{48}$$

with pivot $\mathcal{K}^{0}_{0}(\Omega)$. Later in this Section, we will identify $\mathcal{K}^{m}_{a}(\Omega)$ with a suitable space $hH^\mu(\Sigma(\Omega))$ using the Lie structure on $\Sigma(\Omega)$. Then, Theorem 3.4 of [1] (see also Lemma 3.7 and Proposition 3.9) gives that $\mathcal{C}^\infty_{\mathrm{c}}(\Omega)$ is dense in $\overset{\circ}{\mathcal{K}^{\mu}_{a}}(\Omega)$ and consequently $\mathcal{K}^{-\mu}_{-a}(\Omega)$ is the completion of the space of smooth functions u on Ω satisfying

$$\|u\|_{\mathcal{K}^{-\mu}_{-a}(\Omega)} = \sup_{0\neq v\in\mathcal{C}^\infty_{\mathrm{c}}(\Omega)} \frac{|(u,v)|}{\|v\|_{\mathcal{K}^{\mu}_{a}(\Omega)}} < +\infty. \tag{49}$$

In order to make the identification $\mathcal{K}^{\mu}_{a}(\Omega) \approx hH^\mu(\Sigma(\Omega))$, for suitable h, we introduce next a class of "admissible weights" h.

5.1 The set of weights

If $h > 0$ on Ω, we denote

$$h\mathcal{K}^{\mu}_{a}(\Omega) := \{hu,\ u \in \mathcal{K}^{\mu}_{a}(\Omega)\}, \tag{50}$$

with induced norm, that is $\|hu\|_{h\mathcal{K}^\mu_a(\Omega)} = \|u\|_{\mathcal{K}^\mu_a(\Omega)}$.
A weight h on Ω will be called *admissible* if it is admissible on $\Sigma(\Omega)$. One of the main examples of an admissible weight is η^a_{n-2}, for $a \in \mathbb{R}$. We recall that an admissible weight on $\Sigma(\Omega)$ is a function h of the form $h = \prod_H x_H^{a_H}$, where H ranges through the set of hyperfaces at infinity of $\Sigma(\Omega)$ and $a_H \in \mathbb{R}$. The topology is induced from the topology on the set $\{(a_H)\}$ of exponents.
As discussed after Corollary 4.11, we can always assume $r_\Omega := \prod_H x_H$. In particular, r^a_Ω, $a \in \mathbb{R}$, is the most important example of an admissible weight. It is more suitable to use this weight, which is intimately related to the structure of Lie manifold on $\Sigma(\Omega)$ $(\smallsetminus \partial\text{"}\,\Sigma(\Omega))$ described in Theorem 4.23, instead of η^a_{n-2}. We also have that

$$r^t_\Omega \mathcal{K}^\mu_a(\Omega) = \mathcal{K}^\mu_{a+t}(\Omega), \tag{51}$$

so in a statement about the spaces $h\mathcal{K}^\mu_a(\Omega)$, where h is an admissible weight, we can usually assume that $a = 0$, without loss of generality. These spaces are *weighted Sobolev spaces* in the sense of the following definition. (These spaces are sometimes called *Babuška–Kondratiev spaces.*)

Definition 5.3. Let h be an admissible weight on Ω. The *weighted Sobolev space* of order $\mu \in \mathbb{Z}$ and weight h on Ω is the space $h\mathcal{K}^\mu_0(\Omega)$.

5.2 Sobolev spaces and Lie manifolds

We now identify the weighted Sobolev space $\mathcal{K}^\mu_a(\Omega)$ with $hH^\mu(\Sigma(\Omega))$, for a suitable admissible weight h; more precisely, $h = r_\Omega^{a-n/2}$. The following description of $\mathcal{V}(\Omega)$ for Ω a curvilinear polyhedral domain in $\mathbb{R}^n$ will be useful. It follows readily from Theorem 4.21.

Corollary 5.4. *Let $\Omega \subset \mathbb{R}^n$ be a bounded curvilinear, polyhedral domain. Then*

$$\mathcal{V}(\Omega) = \{\phi_1 r_\Omega \partial_1 + \phi_2 r_\Omega \partial_2 + \ldots + \phi_n r_\Omega \partial_n,\ \textit{where } \phi_j \in \mathcal{C}^\infty(\Sigma(\Omega))\}.$$

We shall denote by

$$\mathrm{Diff}^k_\Omega := \mathrm{Diff}_{\mathcal{V}(\Omega)}(\Sigma(\Omega)) \tag{52}$$

the space of differential operators with coefficients in $\mathcal{C}^\infty(\Sigma(\Omega))$ of order $\leq k$ on $\Sigma(\Omega)$ generated by $\mathcal{V}(\Omega)$. The algebra of differential operators $\mathrm{Diff}^\infty_\Omega$ is an example of the algebra of differential operators considered in 3.3. From the last corollary, we obtain directly the following lemma.

Lemma 5.5. *Let $X_1, X_2, \ldots, X_k$ be smooth vector fields on M. Then*

$$P := r^k_\Omega X_1 X_2 \ldots X_k \in \mathrm{Diff}^k_\Omega.$$

Moreover, Diff^k_Ω *is generated linearly by ϕP, with P as above and $\phi \in \mathcal{C}^\infty(\Sigma(\Omega))$.*

Proof. For $k = 1$, this follows from Lemma 4.16. Next, we have

$$r_\Omega^{k+1} X_0 X_1 \dots X_k = r_\Omega X_0 r_\Omega^k X_1 \dots X_k - k X_0(r_\Omega) r_\Omega^k X_1 \dots X_k.$$

The fact that $P \in \mathrm{Diff}_\Omega^k$ then follows by induction, since $X_0(r_\Omega) \in \mathcal{C}^\infty(\Sigma(\Omega))$, by Lemma 4.14.
Conversely, we can similarly check by induction (using the same identity above) that the product $r_\Omega X_1 r_\Omega X_2 \dots r_\Omega X_k$ can be written as a linearly combination of differential operators of the form ϕP, with $\phi \in \mathcal{C}^\infty(\Sigma(\Omega))$ and P as above. Since $r_\Omega X$ generate $\mathcal{V}(\Omega)$ as a $\mathcal{C}^\infty(\Sigma(\Omega))$–module (see Corollary 5.4 or the second part of Theorem 4.21), the result follows. □

We next provide a different description of the weighted Sobolev spaces $\mathcal{K}_a^\mu(\Omega)$, $\mu \in \mathbb{Z}_+$. For a multiindex α, we denote

$$(r_\Omega \partial)^\alpha := (r_\Omega \partial_1)^{\alpha_1} (r_\Omega \partial_2)^{\alpha_2} \dots (r_\Omega \partial_n)^{\alpha_n}. \tag{53}$$

Theorem 5.6. *Let $\Omega \subset \mathbb{R}^n$ be a bounded curvilinear, stratified polyhedral domain and*

$$\|u\|_{\mu,a}^2 := \sum_{|\alpha| \leq \mu} \|r_\Omega^{-a} (r_\Omega \partial)^\alpha u\|_{L^2(\Omega)}^2.$$

Then $\|u\|_{\mu,a}$ is equivalent to $\|u\|_{\mathcal{K}_a^\mu(\Omega)}$ of Definition 5.2. In particular,

$$\mathcal{K}_a^\mu(\Omega) = \{u, \, \|u\|_{\mu,a} < \infty\}.$$

Proof. We have that

$$\begin{aligned} u \in \mathcal{K}_a^\mu(\Omega) \ &\Leftrightarrow r_\Omega^{|\alpha|-a} \partial^\alpha u \in L^2(\Omega) \quad \text{for all } |\alpha| \leq \mu \quad \text{by Proposition 4.9} \\ &\Leftrightarrow r_\Omega^{-a} (r_\Omega \partial)^\alpha u \in L^2(\Omega) \quad \text{for all } |\alpha| \leq \mu \quad \text{by Proposition 5.5.} \end{aligned}$$

Above the corresponding square integrability conditions define the topology on the indicated spaces. Therefore $\Leftrightarrow$ also means that the topologies are the same. □

We are in position to identify the spaces $\mathcal{K}_a^\mu$ with Sobolev spaces on Lie manifolds. If Ω is a bounded curvilinear, stratified polyhedral domain, we let

$$\mathfrak{O}_0 := \Sigma(\Omega) \smallsetminus \partial'' \Sigma(\Omega) = \Omega \cup \partial' \Sigma(\Omega) = \kappa^{-1}(\overline{\Omega} \smallsetminus \Omega^{(n-2)}),$$

as in Theorem 4.23. Since $(\mathfrak{O}_0, \mathfrak{O} := \Sigma(\Omega), \mathcal{V}(\Omega))$ is a Lie manifold with boundary by the same theorem, the definitions of Sobolev spaces on Lie manifolds (with or without boundary) of Subsection 3.5 provide us with natural spaces $H^s(\Sigma(\Omega)) = H^s(\mathfrak{O}) = H^s(\mathfrak{O}_0)$ and $H^s(\partial' \Sigma(\Omega)) = H^s(\partial \mathfrak{O}_0)$. For the last equality we used that the boundary of $\mathfrak{O}_0$ is $\partial' \Sigma(\Omega)$.

Proposition 5.7. *Let Ω be an n-dimensional, bounded curvilinear, stratified polyhedral domain and let h be an admissible weight on Ω. We have an equality*

$$h\mathcal{K}_a^\mu(\Omega) = hr_\Omega^{a-n/2}H^\mu(\Sigma(\Omega)), \quad \mu \in \mathbb{Z}.$$

Proof. This is again a local statement. We can therefore assume that $\Omega \subset \mathbb{R}^n$. Furthermore, it is enough to prove the statement in the case $h = 1$, since the weight h does not enter into the condition on derivatives in the definition 50 of weighted spaces. Equation (51) and Proposition 4.9 show that we can also assume $a = 0$. Recall from Lemma 3.7 that the spaces $H^k(\Sigma(\Omega))$ are defined using $L^2(\Sigma(\Omega))$. In turn, $L^2(\Sigma(\Omega))$ is defined using the volume element of a compatible metric. A typical compatible metric is $r_\Omega^{-2}g_e$, where g_e is the Euclidean metric. Therefore the volume element on $\Sigma(\Omega)$ is $r_\Omega^{-n}dx$, where dx is the Euclidean volume element. In particular, $v \in L^2(\Omega) \Leftrightarrow v \in r_\Omega^{-n/2}L^2(\Sigma(\Omega))$. We notice next that $r_\Omega^{-t}(r_\Omega\partial)^\alpha r_\Omega^t - (r_\Omega\partial)^\alpha$ is a linear combination with $\mathcal{C}^\infty(\Sigma(\Omega))$–coefficients of monomials $(r_\Omega\partial)^\beta$, with $|\beta| < |\alpha|$, by the second part of Lemma 4.14. From this observation we obtain

$$\begin{aligned} u \in \mathcal{K}_0^\mu(\Omega) &\Leftrightarrow (r_\Omega\partial)^\alpha u \in L^2(\Omega) \quad \text{for all } |\alpha| \le \mu \quad \text{by Theorem 5.6} \\ &\Leftrightarrow (r_\Omega\partial)^\alpha u \in r_\Omega^{-n/2}L^2(\Sigma(\Omega)) \quad \text{for all } |\alpha| \le \mu \\ &\Leftrightarrow (r_\Omega\partial)^\alpha r_\Omega^{n/2}u \in L^2(\Sigma(\Omega)) \quad \text{for all } |\alpha| \le \mu \\ &\Leftrightarrow u \in r_\Omega^{-n/2}H^\mu(\Sigma(\Omega)). \end{aligned}$$

This proves that $\mathcal{K}_a^\mu(\Omega) = r_\Omega^{a-n/2}H^\mu(\Sigma(\Omega))$ for $\mu \in \mathbb{Z}_+$. For $\mu \in \mathbb{Z}_-$, we observe that, for $(\mathfrak{O}, \mathfrak{O}_0, \mathcal{V})$ a Lie manifold with boundary in a manifold with corner $\mathfrak{M}$, the set of restrictions of distributions $u \in H^{-\mu}(\mathfrak{M})$ to $\mathfrak{O}_0$ is the dual of the closure of $\mathcal{C}_c^\infty(\mathfrak{O}_0)$ in $H^{-\mu}(\mathfrak{M})$. Hence

$$\mathcal{K}_0^{-\mu}(\Omega) := \overset{\circ}{\mathcal{K}_a^\mu}(\Omega)^* = \big(r_\Omega^{-n/2}\overset{\circ}{H}{}^\mu(\Sigma(\Omega))\big)^* = r_\Omega^{-n/2}H^{-\mu}(\Sigma(\Omega)).$$

The proof is concluded. □

The identification given in Proposition 5.7 above allows to define weighted spaces on the boundary $h\mathcal{K}_a^m(\partial\Omega)$. We recall that the closure of a hyperface of a curvilinear, stratified polyhedral domain Ω need not be contained in any smooth $n-1$ manifold. Consequently, we utilize the desingularization $\Sigma(\Omega)$. In the special case that $\Omega \subset \mathbb{R}^n$ is a (bounded) convex, stratified polyhedron that in addition has straight faces (*i.e.,* each connected component $D_j^{(l)}$ of $\Omega^{(l)} \smallsetminus \Omega^{(l-1)}$, $l = 1, \ldots, n-1$ is contained in an affine space $V_j^{(l)}$ of dimension l), for example an n-simplex, we can more simply define the spaces on the boundary as follows:

$$\mathcal{K}_a^\mu(D_j^{(n-1)}) = \{u \in L^2_{\mathrm{loc}}(D_j^{(n-1)}),\ r_\Omega^{k-a}X_1\ldots X_k u \in L^2(D_j^{(n-1)}),\ 0 \le k \le l\},$$

for all choices of vector fields X_j in a basis of the linear space containing $D_j^{(n-1)}$. Then for any admissible weight h,

$$h\mathcal{K}_a^\mu(\partial\Omega) = \{hu,\ u \in L^2_{\text{loc}}(\partial\Omega),\ u|_{D_j^{(n-1)}} \in \mathcal{K}_a^\mu(D_j^{(n-1)}),\ \text{ for all } j\}. \tag{54}$$

In the general case of a curvilinear, stratified polyhedral domain, we exploit the structure of Lie manifold on $\Sigma(\Omega)$, following the notation of Proposition 5.7.

Definition 5.8. Let Ω be a bounded, curvilinear, stratified polyhedral domain. Then we define

$$h\mathcal{K}_a^\mu(\partial\Omega) := hr_\Omega^{a-(n-1)/2} H^\mu(\partial'\Sigma(\Omega)),$$

for any admissible weight h.

Note that on each hyperface, the natural weight is the distance to the boundary of that face, not the distance to the set of singular boundary points of that face. The spaces $\mathcal{K}_{-a}^{-\mu}(\partial\Omega)$ are defined to be the duals of $\mathcal{K}_a^\mu(\partial\Omega)$ with pivot $L^2(\partial\Omega)$. For reasons that will be explained later, we do not have to restrict to functions with vanishing trace when studying weighted Sobolev spaces on the boundary. In particular, the usual difficulties that appear in the treatment of Sobolev spaces of fractional order on smooth, bounded domains [49], do not arise when studying the weighted Sobolev spaces on $\partial\Omega$, and we can define the spaces $\mathcal{K}_a^s(\partial\Omega)$, with $s \notin \mathbb{Z}$, by complex interpolation. A similar attempt at defining $\mathcal{K}_a^s(\Omega)$, with $s \in \mathbb{Z} + 1/2$, would lead to the usual difficulties encountered in the case of smooth domain [49].
We next prove a trace theorem, generalizing the corresponding well-known result for smooth domains. Let $\mathcal{C}_c^\infty(\Omega)$ be the space of compactly supported functions on the open set Ω.

Theorem 5.9. *The restriction* $\mathcal{C}_c^\infty(\overline{\Omega}\smallsetminus\Omega^{(n-2)}) \ni u \to u|_{\partial\Omega} \in \mathcal{C}_c^\infty(\partial\Omega\smallsetminus\Omega^{(n-2)})$ *extends to a continuous, surjective map*

$$Tr:\ \mathcal{K}_a^\mu(\Omega) \to \mathcal{K}_{a-1/2}^{\mu-1/2}(\partial\Omega), \quad \mu \ge 1.$$

Moreover, $\mathcal{C}_c^\infty(\Omega)$ *is dense in the kernel of this map if* $\mu = 1$*. Similarly, the normal derivative* ∂_ν *extends to a continuous, surjective map*

$$\partial_\nu:\ \mathcal{K}_a^\mu(\Omega) \to \mathcal{K}_{a-3/2}^{\mu-3/2}(\partial\Omega), \quad \mu \ge 1.$$

The result is a consequence of similar results for Lie manifolds contained in Theorems 3.4 and 3.7 of [1] recalled here in Proposition 3.9. For the normal derivative, we also use the fact that the rescaled normal vector $r_\Omega\nu$ extends to a smooth vector field, first on the boundary of $\Sigma(\Omega)$, and then on the whole of $\Sigma(\Omega)$. The rescaled normal vector is then a unit normal vector for the boundary of $\Sigma(\Omega)$.

Proof. The map $H^\mu(\Sigma(\Omega)) \to H^{\mu-1/2}(\partial'\Sigma(\Omega))$, where we follow the notation of Proposition 5.7, is well defined, continuous, and surjective by Proposition 3.9. Proposition 5.7 then shows that the map

$$h\mathcal{K}_a^\mu(\Omega) = hr_\Omega^{a-n/2} H^\mu(\Sigma(\Omega)) \to hr_\Omega^{a-n/2} H^{\mu-1/2}(\partial\Sigma(\Omega)) = h\mathcal{K}_{a-1/2}^{\mu-1/2}(\partial\Omega)$$

is also well defined, continuous, and surjective.
The density of $\mathcal{C}_c^\infty(\Omega)$ in the subspace of elements in $h\mathcal{K}_a^1(\Omega)$ with trace zero also follows from Proposition 3.9 and Proposition 5.7. □

6 Proofs

In this section, we establish the main results of the paper, Theorems 1.1, 1.2, 1.3, using material from previous sections. We first discuss some results on the behavior of differential operators on the spaces $h\mathcal{K}_a^m(\Omega)$.

6.1 Differential operators

We recall that the algebra $\mathrm{Diff}_\Omega^\infty$ is the natural algebra of differential operators on Ω associated to the Lie algebra of vector fields $\mathcal{V}(\Omega)$, namely, it is generated as an algebra by $X \in \mathcal{V}(\Omega)$ and $\phi \in \mathcal{C}^\infty(\Sigma(\Omega))$. (This algebra was used also in Equation (52) and in Subsection 3.3.)

Proposition 6.1. *Let P be a differential operator of order m on a manifold M with smooth coefficients. Let $\Omega \subset M$ be a curvilinear, stratified polyhedral domain. Then P maps $h\mathcal{K}_a^\mu(\Omega)$ to $h\mathcal{K}_{a-m}^{\mu-m}(\Omega)$ continuously, for any admissible weight h and any $\mu \in \mathbb{Z}$. Moreover, the resulting family $h^{-\lambda}Ph^\lambda : \mathcal{K}_a^\mu(\Omega) \to \mathcal{K}_{a-m}^{\mu-m}(\Omega)$ of bounded operators depends continuously on λ.*

Before proceeding with the proof, we discuss a corollary, which will be relevant in showing that Theorems 1.2 and 1.3 hold. Following the notation of those theorems, below $\mathcal{W}_\mu(\Omega)$ represents the set of admissible weights h such that the map $\tilde{P}(u) := (Pu, u|_{\partial_D\Omega}, D_\nu^P u|_{\partial_N\Omega})$ is an isomorphism $\{\bigoplus_{j=1}^N h\mathcal{K}_1^{\mu+1}(\Omega_j) \cap h\mathcal{K}_1^1(\Omega);\ u^+ = u^-,\ D_\nu^P u^+ = D_\nu^P u^- \text{ on } \Gamma\} \simeq \bigoplus_{j=1}^N h\mathcal{K}_{-1}^{\mu-1}(\Omega_j) \oplus h\mathcal{K}_{1/2}^{\mu+1/2}(\partial_D\Omega) \oplus h\mathcal{K}_{-1/2}^{\mu-1/2}(\partial_N\Omega)$.

Proposition 6.2. *The set $\mathcal{W}_\mu(\Omega)$ is open.*

Proof. This follows directly from Proposition 6.1. Indeed, the family $P : \bigoplus_{j=1}^N h\mathcal{K}_1^{\mu+1}(\Omega_j) \cap h\mathcal{K}_1^1(\Omega) \to h\mathcal{K}_{-1}^{\mu-1}(\Omega)$ is unitarily equivalent to $h^{-1}Ph : \bigoplus_{j=1}^N \mathcal{K}_1^{\mu+1}(\Omega_j) \cap \mathcal{K}_1^1(\Omega) \to \mathcal{K}_{-1}^{\mu-1}(\Omega)$. The result then follows since the set of invertible operators is open. □

For the proof of Proposition 6.1, we observe that if $\Omega \subset \mathbb{R}^n$, the principal symbol of $(r_\Omega \partial)^\alpha$ is $(\imath\xi)^\alpha$. This result follows from the definition of the principal symbol in [2, 1] and from Corollary 5.4. (The reader can just assume $\sigma\big((r_\Omega\partial)^\alpha\big) = (\imath\xi)^\alpha$ by definition.)

Corollary 6.3. *Let P be a differential operator of order m on M with smooth coefficients. Then*

(i) $P_0 := r_\Omega^m P \in \mathrm{Diff}_\Omega$*;*

(ii) P *is uniformly strongly elliptic if, and only if,* $r_\Omega^m P$ *is uniformly strongly elliptic in* Diff_Ω^m*;*

(iii) $h^\lambda P h^{-\lambda}$ *depends continuously on* λ*;*

(iv) P *maps* $h\mathcal{K}_a^\mu(\Omega) \to h\mathcal{K}_{a-m}^{\mu-m}(\Omega)$ *continuously.*

Proof. The relation $r_\Omega^m P \in \mathrm{Diff}_\Omega^m$ was proved as part of Lemma 5.5. Strong ellipticity is a local property, so we can assume $\Omega \subset \mathbb{R}^n$. The proof of Lemma 5.5 shows that P and $r_\Omega^m P$ have the same principal symbol. Therefore they are elliptic (or strongly elliptic) at the same time.

For any $X \in \mathcal{V}$ and any defining function x of some hyperface at infinity of $\Sigma(\Omega)$, we have that $x^\lambda X x^{-\lambda} = X - \lambda x^{-1} X(x)$. Since $x^{-1}X(x)$ is a smooth function (as X is tangent to the face defined by x), we see that $x^\lambda X x^{-\lambda} \in \mathrm{Diff}_\Omega^1$ and depends continuously on λ, establishing (iii). It also shows, in particular, that Diff_Ω^k is conjugation invariant with respect to defining functions of hyperfaces at infinity (Equation (28)). We can therefore assume that $h = 1$.

Since $(\Sigma(\Omega), \mathcal{V}(\Omega))$ is a Lie manifold with boundary (Theorem 4.23) any $P_0 \in \mathrm{Diff}_\Omega^k$ maps $H^\mu(\Sigma(\Omega)) \to H^{\mu-k}(\Sigma(\Omega))$ continuously. (This simple property, proved in [1], is an immediate consequence of the definitions.) The continuity of $P = r_\Omega^{-m} P_0 : \mathcal{K}_a^\mu(\Omega) \to \mathcal{K}_{a-m}^{\mu-m}(\Omega)$ then follows using also the fact that multiplication by r_Ω^{-m} defines an isometry $\mathcal{K}_a^{\mu-m}(\Omega) \simeq \mathcal{K}_{a-m}^{\mu-m}(\Omega)$. □

6.2 A weighted Hardy–Poincaré's inequality

The stepping stones in the proof of our main result on the solvability of the mixed boundary value/interface problem (6), Theorem 1.2, consist of

(i) a Hardy–Poincaré type inequality (Theorem 6.4);

(ii) the regularity result for polyhedra (Theorem 1.1).

We address the Hardy-Poincaré inequality first and turn to the proof of the regularity result, which is more general and of independent interest in the next subsection. Let $dx = dx_1 dx_2 \dots dx_n$ denote the standard volume element in $\mathbb{R}^n$. We continue to denote by Ω a curvilinear, stratified polyhedral domain satisfying hypotheses (3)–(5).

Theorem 6.4. *Let Ω be a bounded, connected, curvilinear, stratified polyhedral domain $\Omega \subset M$. Assume that $\partial_D\Omega \neq \emptyset$ and $\partial_N\Omega$ does not contain any two adjacent hyperfaces. Then there exists a constant $\kappa_\Omega > 0$, depending only on the polyhedral structure of Ω, such that*

$$\|u\|^2_{\mathcal{K}^0_1(\Omega)} := \int_\Omega \frac{|u(x)|^2}{\eta_{n-2}(x)^2}\, dx \leq \kappa_\Omega \int_\Omega |\nabla u(x)|^2\, dx, \tag{55}$$

for any function $u \in H^1_{\text{loc}}(\Omega)$ such that $u|_{\partial_D\Omega} = 0$.

Above, if u/η_{n-2} is not square integrable, the statement of the theorem is understood to mean that ∇u is not square integrable either. By Propositions 4.9 and 4.10, we can replace the distance to the singular set η_{n-2} with the more regular weight r_Ω.
The proof proceeds by induction on the dimension n. We discuss first the case $n = 2, 3$.
The case $n = 2$. In view of the local nature of the definition of a curvilinear, stratified polygonal domain, Definition 2.6, it will be sufficient to have the Hardy-Poincaré inequality in a sector. By abuse of notation, we shall write $u(r,\theta) := u(r\cos\theta, r\sin\theta)$ for a function $u(x_1,x_2)$ expressed in polar coordinates. The proof of the following elementary lemma can be found in e.g. [62][Subsection 2.3.1]. See also [40].

Lemma 6.5. *Let $\mathcal{C} = \mathcal{C}_R(\alpha,\beta) := \{(r\cos\theta, r\sin\theta) \in \mathbb{R}^2, 0 < r < R, \beta < \theta < \alpha\}$, $0 < \alpha - \beta < 2\pi$. Then*

$$\int_{\mathcal{C}} \frac{|u|^2}{r^2}\, dx \leq \frac{\pi^2}{(\alpha-\beta)^2} \int_{\mathcal{C}} |\nabla u|^2 dx$$

for any $u \in H^1_{\text{loc}}(\mathcal{C})$ satisfying $u(r,\theta) = 0$ if $\theta = \beta$ or $\theta = \alpha$. The same result holds if $\mathcal{C}$ is the disjoint union of domains $\mathcal{C}_R(\alpha,\beta)$, for different values of R, α, and β.

From the Lemma above, we obtain the case $n = 2$ in Theorem 6.4, the first step in our induction proof. A detailed proof can be found e.g. in the papers [15, 56].

Lemma 6.6. *Let Ω be a connected, curvilinear, stratified polygonal domain in a two dimensional manifold M. Assume that $\partial_D\Omega \neq \emptyset$ and $\partial_N\Omega$ does not contain any two adjacent sides of Ω. Fix an arbitrary metric g on M and let $\eta_0(z)$ be the distance from z to the vertices of Ω. Then there exists a constant $\kappa_\Omega > 0$ such that*

$$\int_\Omega \frac{|u(w)|^2}{\eta_0(w)^2}\, dz \leq \kappa_\Omega \int_\Omega |\nabla u(w)|^2 dz$$

for any $u \in H^1_{\text{loc}}(\Omega)$ satisfying $u = 0$ on $\partial_D\Omega$.

The case $n = 3$. The proof of Theorem 6.4 for $n = 3$ combines the methods used in the previous two Lemmata and the inequality for the case $n = 2$. We give a self-contained proof again, especially because the induction step in the general case is very similar. The general case $n > 3$ will be completed using Proposition 4.10.

Proof. Let us fix, for any $p \in \partial\Omega$, a neighborhood V_p of p in M and a diffeomorphism $\phi_p : V_p \to U = B^{3-l} \times B^l$ as in Definition 2.8, where $l = \ell(p)$. We denote $\mathcal{C} := \phi_p(V_p \cap \Omega)$. We shall use the notation ω_p introduced in that definition. By decreasing V_p, if necessary, we may assume that ϕ_p extends to a diffeomorphism defined in a neighborhood of $\overline{V}_p$ in $\mathbb{R}^3$.
Since $\eta_{n-2} = \eta_1$ is the distance to the singular set $\Omega^{(1)}$ of Ω, we need only discuss two cases:

(a) $l = \ell(p) = 0$, *i.e.,* p is a true or artificial vertex;

(b) $l = \ell(p) = 1$, *i.e.,* p belongs to a true or artificial edge.

If $l = 0$, we denote by $\psi_0(x')$ the distance from a point $x' \in \omega_p \subset S^2$ to the vertices of ω_p and let $r_p(w) = \rho\psi_0(x')$, if $\phi_p(w) = \rho x'$, where $0 < \rho$ and $x' \in \omega_p$. If $l = 1$, we let $r_p(w) = r$ if $\phi_p(w) = (r\cos\theta, r\sin\theta, z)$, where $0 < r$, $0 < \theta < \alpha$, and $z \in \mathbb{R}$. (These definitions agree with the general definition of r_Ω given in (36) with $r_p = r_\alpha$ given in (35).) As before, the function $\eta_1(x)/r_p(x)$ is bounded for any p, provided that we choose the neighborhoods V_p small enough, uniformly in p. Below, we shall write $u(x)$ instead of $u(\phi_p^{-1}(x))$, by abuse of notation.
If $l = 1$, $\mathcal{C} = \mathcal{C}' \times (-1, 1)$, so that we exploit the Hardy-Poincaré inequality in a sector of Lemma 6.5. In fact

$$\int_{V_p\cap\Omega} \frac{|u(w)|^2}{\eta_1(w)^2}\, dw = C \int_{\Omega\cap V_p} \frac{|u(x)|^2}{r^2} \left|\frac{\partial w}{\partial x}\right| dx \leq C \int_{\mathcal{C}} \frac{|u(x)|^2}{r^2}\, dx. \qquad (56)$$

so that we obtain

$$\begin{aligned}\int_{\mathcal{C}} \frac{|u(x)|^2}{r^2}\, dx &= \int_{-1}^{1} \left(\int_{\mathcal{C}'} \frac{|u(x)|^2}{r^2}\, dx_1 dx_2\right) dx_3 \\ &\leq \int_{-1}^{1} \left(\int_{\mathcal{C}'} |\nabla_{(x_1,x_2)} u(x)|^2\, dx_1 dx_2\right) dx_3 \leq \int_{-1}^{1} \left(\int_{\mathcal{C}'} |\nabla u(x)|^2\, dx_1 dx_2\right) dx_3 \\ &\leq C \int_{V_p\cap\Omega} |\nabla u(w)|^2\, dw. \qquad (57)\end{aligned}$$

We perform a similar calculation on $V_p \cap \Omega$ when $l = 0$, using spherical coordinates instead. Recall that $\mathcal{C} = \phi_p(V_p \cap \Omega) = \{\rho x',\ 0 < \rho < 1,\ x' \in \omega_p\}$, hence following (56) and using that $C\eta_1(x) \geq \rho\psi_0(x)$ The inequality

$$\int_{V_p\cap\Omega} \frac{|u(w)|^2}{\eta_1(w)^2}\, dw \leq C \int_{\mathcal{C}} \frac{|u(x)|^2}{\rho^2\psi_0(x')^2}\, dx, \quad x = \rho x',\ |x'| = 1, \qquad (58)$$

Next, we observe that $\nabla u(\rho x') = \rho^{-1}\nabla' u(\rho x') + \partial_\rho u(\rho x')$, with ∇' the gradient of a function defined on ω_p, so that $|\nabla' u(\rho x')|^2 \leq \rho^2 |\nabla u(\rho x')|$, which gives

$$\int_{\mathcal{C}} \frac{|u(x)|^2}{\rho^2 \psi_0(x)^2}\, dx = \int_0^1 \left(\int_{\omega_p} \frac{|u(\rho x')|^2}{\psi_0^2} dx' \right) d\rho$$
$$\leq C \int_0^1 \left(\int_{\omega_p} |\nabla' u(\rho x')|^2 dx' \right) d\rho \leq C \int_0^1 \left(\int_{\omega_p} \rho^2 |\nabla u(\rho x')|^2 dx' \right) d\rho$$
$$\leq C \int_{V_p \cap \Omega} |\nabla u(w)|^2\, dw. \quad (59)$$

We can rewrite the above inequalities simply as

$$\int_{V_p \cap \Omega} \frac{|u(w)|^2}{\eta_1(w)^2}\, dz \leq C_p \int_{V_p \cap \Omega} |\nabla u(w)|^2\, dz \leq C_p \int_{\Omega} |\nabla u(w)|^2\, dw, \quad (60)$$

where the constant C_p depends on the point $p \in \Omega^{(1)}$ but not on u.
To conclude the proof, as before we cover the singular set $\Omega^{(1)}$ with finitely many sets $V_p = V_{p_k}$. Let $C_0 > \eta_1^{-2}$ *outside* the union of the sets V_{p_k}. Let $\kappa_\Omega = C_0 C_\Omega + \sum C_{p_k}$, where C_Ω is the standard Poincaré inequality constant for the domain Ω. We add all inequalities (60) for $p = p_k$ and combine it with the Poincaré inequality to get

$$\int_{\Omega} \frac{|u(w)|^2}{\eta_1^2(w)} dw \leq \kappa_\Omega \int_\Omega |\nabla u(w)|^2 dw. \quad (61)$$

The proof of Theorem 6.4 is now complete for $n = 3$. ☐

The general case $n > 3$. To conclude the proof of theorem 6.4, we need only establish the induction step. The induction step follows very closely the proof of the case $n = 3$. The only delicate point is showing that the ratio $\eta_{n-2}(x)/r_\alpha(x)$ is bounded on $\overline{\Omega}$, where η_{n-2} is the distance to the singular set $\Omega^{(n-2)}$ of Ω and r_α is as in Equation 35. This fact was established in Proposition 4.9.
We conclude with an immediate corollary of Theorem 6.4, which will be used in the proof of Theorem 1.2

Corollary 6.7. *There exists a constant $\kappa'_\Omega > 0$, depending only on Ω, such that*

$$\frac{1}{\kappa'_\Omega} \|u\|^2_{\mathcal{K}^1_1(\Omega)} \leq \int_\Omega |\nabla u(x)|^2\, dx\,,$$

for any function $u \in H^1_{\text{loc}}(\Omega)$ such that $u|_{\partial_D \Omega} = 0$, if $\partial_D \Omega \neq \emptyset$ and $\partial_N \Omega$ does not contain any two adjacent hyperfaces.

6.3 Proofs of the main results

In this subsection, we finally tackle the proofs of the main results of the paper. We first show how the proof of the regularity property for the mixed boundary value/interface problem (6), Theorem 1.1 can be obtained from the results of [1] and the theory developed in Section 4. The following result was proved in [1].

Theorem 6.8. *Let $(\mathfrak{M}, \mathcal{V})$ be a Lie manifold with boundary and $P_0 := r_\Omega^2 P \in \mathrm{Diff}^2(\mathfrak{M})$ be a second order, uniformly strongly elliptic operator. Let h be an admissible weight and $u \in hH^1(\mathfrak{M})$ be such that $Pu \in hH^{\mu-1}(\mathfrak{M})$ and $u|_{\partial\mathfrak{M}} \in hH^{\mu+1/2}(\partial\mathfrak{M})$, $\mu \in \mathbb{Z}_+$. Then $u \in hH^{\mu+1}(\mathfrak{M})$ and*

$$\|u\|_{hH^{\mu+1}(\mathfrak{M})} \leq C\big(\|Pu\|_{hH^{\mu-1}(\mathfrak{M})} + \|u\|_{hH^0(\mathfrak{M})} + \|u|_{\partial\Omega}\|_{hH^{\mu+1/2}(\partial\mathfrak{M})}\big). \quad (62)$$

For mixed boundary value/interface problems we need the following extension of this theorem, which is proved exactly in the same way.

Theorem 6.9. *Let $(\mathfrak{M}, \mathcal{V})$ be a Lie manifold with boundary and $P_0 = r_\Omega^2 P \in \mathrm{Diff}^2(\mathfrak{M})$ be a second order, uniformly strongly elliptic operator with jump discontinuities on sub Lie manifolds of $\mathfrak{M}$ that partition it into subsets $\mathfrak{M}_j$. Assume that $\partial\mathfrak{M} = \partial_D\mathfrak{M} \cup \partial_N\mathfrak{M}$ is a disjoint decomposition into* open*, disjoint subsets. Let h be an admissible weight and $u \in hH^1(\mathfrak{M})$ be such that $Pu \in hH^{\mu-1}(\mathfrak{M}_j)$ and $u|_{\partial\mathfrak{M}} \in hH^{\mu+1/2}(\partial\mathfrak{M})$, $\mu \in \mathbb{Z}_+$. Then $u \in hH^{\mu+1}(\mathfrak{M}_j)$ and*

$$\|u\|_{hH^{\mu+1}(\mathfrak{M}_j)} + \|u\|_{hH^1(\mathfrak{M})} \leq C\big(\sum_k \|Pu\|_{hH^{\mu-1}(\mathfrak{M}_k)} + \|u\|_{hH^0(\mathfrak{M})} \\ + \|u|_{\partial\Omega}\|_{hH^{\mu+1/2}(\partial_D\mathfrak{M})} + \|D_\nu^P u|_{\partial\Omega}\|_{hH^{\mu-1/2}(\partial_N\mathfrak{M})}\big).$$

Theorem 1.1 then follows by applying the above theorem to $P_0 := r_\Omega^2 P$, which is strongly elliptic by Corollary 6.3(ii), and using the identifications of Proposition 5.7 and Definition 5.8.

We now prove Theorem 1.2 assuming the results stated in the previous subsection. The proof of Theorem 1.3 is completely similar.

Remark 6.10. In the statement of Theorems 1.2 and 1.3, the spaces $\mathcal{K}_1^{\mu+1}(\Omega_j)$ are defined intrinsically, without reference to Ω. However, the interface Γ is assumed smooth for well-posedness in this paper (more general conditions on Γ were for example considered in [48]) and the points where Γ intersects $\partial\Omega$, necessarily transversely, are included in the singular sets $\Omega^{(n-2)}$ of Ω; consequently, r_Ω is equivalent to r_{Ω_j} in each Ω_j.

Proof. We first notice that Theorem 5.9 allows us to reduce the proof to the case $g_D = 0$.

We continue to denote with $\mathcal{W}_\mu(\Omega)$ the set of weights such that the operator $\tilde{P}$, defined below, is an isomorphism

$$\tilde{P} := (Pu, u|_{\partial_D\Omega}, D^P_\nu u|_{\partial_N\Omega}) :$$
$$\{u \in \bigoplus_{j=1}^N h\mathcal{K}^{\mu+1}_1(\Omega_j) \cap h\mathcal{K}^1_1(\Omega); u|_{\partial_D\Omega} = 0, u^+ = u^-, D^P_\nu u^+ = D^P_\nu u^- \text{ on } \Gamma\}$$
$$\to \bigoplus_{j=1}^N h\mathcal{K}^{\mu-1}_{-1}(\Omega_j) \oplus h\mathcal{K}^{\mu-1/2}_{-1/2}(\partial_N\Omega), \quad (63)$$

which is an open set by Proposition 6.2. Therefore, it is enough to show that $1 \in \mathcal{W}_\mu(\Omega)$ to complete the proof.
For solvability, we consider the case $\mu = 0$. For $\mu = 0$, the problem (6) is interpreted in the weak sense (11), using that $\mathcal{K}^1_1(\Omega) \subset H^1(\Omega)$. More precisely, we let

$$\mathcal{H} := \{u \in \mathcal{K}^1_1(\Omega),\ u = 0 \text{ on } \partial_D\Omega\}, \quad (64)$$

and we define the weak solution u of Equation (11) with $g_D = 0$ as the unique $u \in \mathcal{K}^1_1(\Omega)$ satisfying $u = 0$ on $\partial_D\Omega$ in trace sense and

$$B_P(u, v) = \Phi(v) \quad \text{for all } \ v \in \mathcal{H}, \quad (65)$$

where the element $\Phi \in \mathcal{H}^*$ is defined by $\Phi(u) = \int_\Omega fu\,dx + \int_{\partial_N\Omega} g_N u\,dS(x)$, this last integral being the pairing between $\mathcal{K}^{1/2}_{1/2}(\partial\Omega)$ and $\mathcal{K}^{-1/2}_{-1/2}(\partial\Omega)$. Here, we have employed the trace property, Theorem 5.9. We will establish the existence and uniqueness of u by using the Lax-Milgram Lemma and coercive estimates for P in weighted Sobolev spaces, which in turn follow from the (uniform) strong ellipticity of P and the Hardy-Poincaré inequality of Theorem 6.4. This result gives the first step of the proof, that is, $1 \in \mathcal{W}_0(\Omega)$. We refer to [26] for the version of the Lax–Milgram lemma needed in this proof, where P contains lower-order terms.
Indeed, the sesquilinear form B is continuous on $\mathcal{H} \times \mathcal{H}$ by Proposition 6.1. Furthermore, assumptions 8 on the coefficients A_{jk}, B_j, and C of the operator P, together with Corollary 6.7 imply the following inequality for the real part of $B(u, v)$:

$$Re\big(Pu, u\big) = \int_\Omega \Big(Re \sum_{j,k=1}^n A_{jk}\partial_k u \overline{\partial_j u}\Big)\,dx + \big((2C - \sum_j \partial_j B_j)u, u\big)/2$$
$$\geq \epsilon \sum_{j=1}^n \|\partial_j u\|^2 \geq \epsilon \|u\|^2_{\mathcal{K}^1_1(\Omega)} =: \epsilon \|u\|^2_{\mathcal{K}^1_1(\Omega)}, \quad (66)$$

which shows that B is strictly coercive on $\mathcal{H}$.
The assumptions of the Lax-Milgram lemma are therefore satisfied, Hence $P : \mathcal{H} \to \mathcal{H}^*$ is an isomorphism (*i.e.,* P is continuous with continuous inverse), proving that $1 \in \mathcal{W}_0(\Omega)$.

We next consider the case $\mu \geq 1$ and prove that $\mathcal{W}_0(\Omega) \subset \mathcal{W}_\mu(\Omega)$ for any $\mu \in \mathbb{Z}_+$, so that, in particular, $1 \in \mathcal{W}_\mu(\Omega)$. We pick $h \in \mathcal{W}_0(\Omega)$ and observe that by the regularity theorem, Theorem 1.1, the map $\tilde{P}$ of Equation 63 above is surjective. Since this map is also continuous (Proposition 6.1) and injective (because $h \in \mathcal{W}_0(\Omega)$), it is an isomorphism by the open mapping theorem. This observation shows that $\mathcal{W}_0(\Omega) \subset \mathcal{W}_\mu(\Omega)$, for any $\mu \in \mathbb{Z}_+$.
Since we have already proved that $\mathcal{W}_\mu(\Omega)$ is open, the proof is complete. □

Remark 6.11. It seems that it would be more natural to work in the framework of stratified spaces than in the framework of polyhedral domains. For example, if we consider a smooth, bounded domain $\Omega \subset \mathbb{R}^n$ and a submanifold $X \subset \partial\Omega$ of lower dimension, then we can consider $\eta_{n-2}(x)$ to be the distance from x to X. Then Theorem 1.2 remains true, with essentially the same proof, by taking $\Omega^{(n-2)} := X$ in this case.

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The Rank-One Limit of the Fourier-Mukai Transform

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Abstract. We give a formula for the specialization of the Fourier-Mukai transform on a semi-abelian variety of torus rank 1.

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1. Introduction

Let $\pi : \mathcal{X}^\star \to S$ be a semi-abelian variety of relative dimension g over the spectrum S of a discrete valuation ring R with algebraically closed residue field k such that the generic fibre X_η is a principally polarized abelian variety. We assume that $\mathcal{X}^\star$ is contained in a complete rank-one degeneration $\mathcal{X}$. In particular, the special fibre X_0 of $\mathcal{X}$ is a complete variety over k containing as an open part the total space of the $\mathbb{G}_m$-bundle associated to a line bundle $J \to B$ over a $(g-1)$-dimensional abelian variety B. The normalization $\nu : \mathbb{P} \to X_0$ of X_0 can be identified with the $\mathbb{P}^1$-bundle over B associated to J and X_0 is obtained by identifying the zero-section of $\mathbb{P}$ with the infinity-section of $\mathbb{P}$, both isomorphic to B, by a translation. Moreover, X_0 is provided with a theta divisor that is the specialization of the polarization divisor on the generic fibre. If c_η is an algebraic cycle on X_η we can take the Fourier-Mukai transform $\varphi_\eta := F(c_\eta)$ and consider the limit cycle (specialization) φ_0 of φ_η. A natural question is: What is the limit φ_0 of φ_η?

If $q : \mathbb{P} \to B$ denotes the natural projection of the $\mathbb{P}^1$-bundle, the Chow ring $A^*(\mathbb{P})$ of $\mathbb{P}$ is the extension $\mathrm{A}^*(B)[\eta]/(\eta^2 - \eta \cdot q^*c_1(J))$ of the Chow ring $A^*(B)$ of B with $\eta = c_1(O_{\mathbb{P}}(1))$. We consider now cycles with rational coefficients. We denote by c_0 the specialization of the cycle c_η on X_0. We can write c_0 as $\nu_*(\gamma)$ with $\gamma = q^*z + q^*w \cdot \eta$.

Theorem 1.1. *Let c_η be a cycle on X_η with $c_0 = \nu_*(q^*z + q^*w \cdot \eta)$, for $z, w \in \mathrm{A}^*(B)$. The limit φ_0 of the Fourier-Mukai transform $\varphi_\eta = F(c_\eta)$ is given by $\varphi_0 = \nu_*(q^*a + q^*b \cdot \eta)$ with*

$$a = F_B(w) + \sum_{n=0}^{2g-2} \sum_{m=0}^{n} \frac{(-1)^m}{(n+2)!} F_B[(z + w \cdot c_1(J)) \cdot c_1^m(J)] \cdot c_1^{n-m+1}(J)$$

and

$$b=\sum_{n=0}^{2g-2}\sum_{m=0}^{n}\frac{(-1)^m}{(n+2)!}F_B[(((-1)^{n+1}-1)z-w\cdot c_1(J))\cdot c_1^m(J)]\cdot c_1^{n-m}(J)\,,$$

where F_B is the Fourier-Mukai transform on the abelian variety B.

We denote algebraic equivalence by $\stackrel{a}{=}$. The relation $c_1(J)\stackrel{a}{=}0$ implies the following result.

THEOREM 1.2. *With the above notation the limit φ_0 satisfies*

$$\varphi_0\stackrel{a}{=}\nu_*(q^*F_B(w)-q^*F_B(z)\cdot\eta)\,.$$

Note that this is compatible with the fact that for a principally polarized abelian variety A of dimension g the Fourier-Mukai transform satisfies $F_A\circ F_A=(-1)^g(-1_A)^*$.

Beauville introduced in [2] a decomposition on the Chow ring with rational coefficients of an abelian variety using the Fourier-Mukai transform. Theorem 1.2 can be used to deduce non-vanishing results for Beauville components of cycles on the generic fibre of a semi-abelian variety of rank 1; we refer to § 7 for examples.

We prove the theorem by constructing a smooth model $\mathcal{Y}$ of $\mathcal{X}\times_S\mathcal{X}$ to which the addition map $\mathcal{X}^\star\times_S\mathcal{X}^\star\to\mathcal{X}^\star$ extends and by choosing an appropriate extension of the Poincaré bundle to $\mathcal{Y}$. The proof is then reduced to a calculation in the special fibre. We refer to Fulton's book [8] for the intersection theory we use. The theory in that book is built for algebraic schemes over a field. In our case we work over the spectrum of a discrete valuation ring. But as is stated in § 20.1 and 20.2 there, most of the theory in Fulton's book, including in particular the statements we use in this paper, is valid for schemes of finite type and separated over S. However, for us projective space denotes the space of hyperplanes and not lines, which conflicts with Fulton's book, but is in accordance with [10].

2. FAMILIES OF ABELIAN VARIETIES WITH A RANK ONE DEGENERATION

We now assume that R is a complete discrete valuation ring with local parameter t, field of quotients K and algebraically closed residue field k. Suppose that $(\mathcal{X}^\star,\mathcal{L})$ is a semi-abelian variety over $S=\mathrm{Spec}(R)$ such that the generic fibre X_η is abelian and the special fibre X_0^* has torus rank 1; moreover, we assume that $\mathcal{L}$ is a cubical invertible sheaf (meaning that $\mathcal{L}$ satisfies the theorem of the cube, see [7], p. 2, 8) and L_η is ample. In particular, the special fibre of $\mathcal{X}^\star$ fits in an exact sequence

$$1\to T_0\to X_0^*\to B\to 0,$$

where B is an abelian variety over k and T_0 the multiplicative group $\mathbb{G}_m$ over k. The torus T_0 lifts uniquely to a torus T_i of rank 1 over $S_i=\mathrm{Spec}(R/(t^{i+1})$ in $X_i^*=\mathcal{X}^\star\times_S S_i$. The quotient X_i^*/T_i is an abelian variety B_i over S_i. The system $\{B_i\}_{i=1}^{\infty}$ defines a formal abelian variety which is algebraizable, resulting in an abelian scheme $\mathcal{B}$, so that we have an exact sequence of group schemes over S

$$1 \to T \to G \xrightarrow{\pi} \mathcal{B} \to 0,$$

cf. [F-C, p. 34]. We assume now that we are given a line bundle M on $\mathcal{B}$ defining a principal polarization $\lambda : B \to B^t$ and consider $L = \pi^*(M)$. This defines a cubical line bundle on G. The extension G is given by a homomorphism c of the character group $Z \cong \mathbb{Z}$ of T to $\mathcal{B}^t$. The semi-abelian group scheme dual to $\mathcal{X}^\star$ defines a similar extension

$$1 \to T^t \to G^t \to \mathcal{B}^t \to 0$$

and the polarization provides an isomorphism ϕ of the character group Z of T with the character group Z^t of T^t. Now the degenerating abelian variety (i.e. semi-abelian variety) $\mathcal{X}^\star$ over S gives rise to the set of degeneration data (cf. [7], p 51, Thm 6.2, or [1], Def. 2.3):

(i) an abelian variety $\mathcal{B}$ over S and a rank 1 extension G. This amounts to a S-valued point b of $\mathcal{B} = \mathcal{B}^t$.
(ii) a K-valued point of G lying over b.
(iii) a cubical ample sheaf L on G inducing the polarization on $\mathcal{B}$ and an action of $Z = Z^t$ on L_η.

A section $s \in \Gamma(G, L)$ possesses the analogue of a classical Fourier expansion as explained in [7], p. 37. So s can be written uniquely as $s = \sum_{\chi \in Z} \sigma_\chi(s)$, where $\sigma_\chi : \Gamma(G, L) \to \Gamma(\mathcal{B}, M_\chi)$ is a R-linear homomorphism and M_χ is the twist of M by χ: in fact $\pi_*(O_G) = \oplus_\chi O_\chi$ with O_χ the subsheaf consisting of χ-eigenfunctions. (We refer to [7], p. 43; note also the sign conventions there in the last lines.) We have now by the action

$$T^*_{c^t(y)} M \cong M_{\phi(y)} \cong M \otimes O_{\phi(y)}, \qquad y \in Z^t.$$

This satisfies $\sigma_{\chi+1}(s) = \psi(1)\tau(\chi)T_b^*(\sigma_\chi(s))$, where τ is given by a point of $G(K)$ lying over b and ψ is a cubical trivialization of $T^*_{c^t(y)} M_\eta^{-1}$ as in [7], p. 44, Thm. 5.1. We refer to Faltings-Chai's theorem (6.2) of [7], p. 51 for the degeneration data.

The compactification $\mathcal{X}$ of $\mathcal{X}^\star$ is now constructed as a quotient of the action of Z^t on a so-called relatively complete model. Such a relatively complete model $\tilde{P}$ for G can be constructed here in an essentially unique way. If B is trivial (i.e. $\dim(B) = 0$) and if the torus is $T = \mathrm{Spec}(R[z, z^{-1}])$ it is given as the toroidal variety obtained by gluing the affine pieces

$$U_n = \mathrm{Spec}(R[x_n, y_n]), \qquad \text{with} \qquad x_n y_n = t$$

where $G \subset \tilde{P}$ is given by $x_n = z/t^n$, $\quad y_n = t^{n+1}/z$, (cf. [13], also in [7], p. 306). By glueing we obtain an infinite chain $\tilde{P}_0$ of $\mathbb{P}^1$'s in the special fibre. We can 'divide' by the action of Z^t; this is easy in the analytic case, more involved in the algebraic case, but amounts to the same, cf. [13], also [7], p. 55-56.

In the special fibre we find a rational curve with one ordinary double point. If instead we divide by the action of nZ^t for $n > 1$ we find a cycle consisting of n copies of $\mathbb{P}^1$.

In case the abelian part B is not trivial we take as a relatively complete model the contracted (or smashed) product $\tilde{P} \times^T G$ with $\tilde{P}$ the relatively complete model for the case that B is trivial. Call the resulting space $\tilde{P}$. Then $\tilde{P}$ corresponds by Mumford's [loc. cit., p 29] to a polyhedral decomposition of $Z^t \otimes \mathbb{R} = \mathbb{R}$ with Z^t the cocharacter group of T. Then we essentially quotient by the action of Z^t or nZ^t as before and obtain a proper $\mathcal{X} \to S$.
We describe the central fibre X_0 of $\mathcal{X}$. Let b be the k-valued point of $B \cong B^t$ that determines the above $\mathbb{G}_m$-extension. If M denotes a line bundle defining the principal polarization of B we let M_b be the translation of M by b and we set $J = M \otimes M_b^{-1}$ and define the projective bundle $\mathbb{P} = \mathbb{P}(J \oplus \mathcal{O}_B)$ with projection $q : \mathbb{P} \to B$. The bundle $\mathbb{P}$ has two natural sections (with images) $\mathbb{P}_1$ and $\mathbb{P}_2$ corresponding to the projections $J \oplus \mathcal{O}_B \to J$ and $J \oplus \mathcal{O}_B \to \mathcal{O}_B$. We have $\mathcal{O}(\mathbb{P}_1) \cong \mathcal{O}(\mathbb{P}_2) \otimes q^*J$ and $\mathcal{O}(1) \cong \mathcal{O}(\mathbb{P}_1)$ with $\mathcal{O}(1)$ the natural line bundle on $\mathbb{P}$. We denote by $\overline{\mathbb{P}}$ the non-normal variety obtained by gluing the sections $\mathbb{P}_1$ and $\mathbb{P}_2$ under a translation by the point b. The singular locus of $\overline{\mathbb{P}}$ has support isomorphic to B. The line bundle $\tilde{L} = \mathcal{O}(\mathbb{P}_1) \otimes q^*M_b \cong \mathcal{O}(\mathbb{P}_2) \otimes q^*M$ descends to a line bundle $\overline{L}$ on $\overline{\mathbb{P}}$ with a unique ample divisor D, see [14]. The central fibre X_0 of the family $\pi : \mathcal{X} \to S$ is then equal to $\bar{\mathbb{P}}$. The cubical invertible sheaf $\mathcal{L}$ on $\mathcal{X}^\star$ extends (uniquely) to $\mathcal{X}$ and its restriction to the central fibre $\bar{\mathbb{P}}$ is the line bundle $\overline{L}$, see [15].

3. Extension of the addition map

The addition map $\mu : \mathcal{X}^\star \times_S \mathcal{X}^\star \to \mathcal{X}^\star$ of the semi-abelian scheme $\mathcal{X}^\star$ does not extend to a morphism $\mathcal{X} \times_S \mathcal{X} \to \mathcal{X}$, but it does so after a small blow-up of $\mathcal{X} \times_S \mathcal{X}$ as we shall see.
The degeneration data of $\mathcal{X}^\star$ defines (product) degeneration data for $\mathcal{X}^\star \times_S \mathcal{X}^\star$. Indeed, we can take the fibre product of the relatively complete model $\tilde{P}' = \tilde{P} \times_S \tilde{P}$ and this corresponds (e.g. via [13], Corollary (6.6)) to the standard polyhedral decomposition of $\mathbb{R}^2 = (Z^t \otimes \mathbb{R})^2$ by the lines $x = m$ and $y = n$ for $m, n \in \mathbb{Z}$. The special fibre of the model $\tilde{P}'$ is an infinite union of $\mathbb{P}^1 \times \mathbb{P}^1$-bundles over $B \times B$ glued along the fibres over 0 and ∞. The compactified model of $\mathcal{X} \times_S \mathcal{X}$ is obtained by taking the 'quotient' of $\tilde{P}'$ under the action of $Z^t \times Z^t$. This is not regular; for example the criterion of Mumford ([13], p. 29, point (D)]) is not satisfied. We can remedy this by subdividing. For example, by taking the decomposition of $\mathbb{R}^2$ given by the lines $x = m, y = n$ and $x + y = l$ for $m, n, l \in \mathbb{Z}$.
The special fibre of this model is an infinite union of copies of $\mathbb{P}^1 \times \mathbb{P}^1$-bundles over $B \times B$ blown up in the two anti-diagonal sections $(0, \infty) = \mathbb{P}_1 \times \mathbb{P}_2$ and $(\infty, 0) = \mathbb{P}_2 \times \mathbb{P}_1$. This is regular.
Both polyhedral decompositions are invariant under the action of translations $(x, y) \mapsto (x + a, y + b)$ for fixed $a, b \in \mathbb{Z}$. This means that we can form the 'quotient' by $Z^t \times Z^t \cong \mathbb{Z}^2$ (or a subgroup $nZ^t \times nZ^t$) and obtain a completed semi-abelian variety $\mathcal{Y}$ of relative dimension $2g$ over S. We denote by $\epsilon : \mathcal{Y} \to \mathcal{Y}' = \mathcal{X} \times_S \mathcal{X}$ the natural map. We shall write V for Y_0 and $\sigma : \tilde{V} \to V$ for

its normalization. Then $\tilde{V}$ is an irreducible component of the special fibre of $\tilde{P}'$. We denote by $\tau : \tilde{V} \to \mathbb{P} \times \mathbb{P}$ the blow up map and by E_{12} and E_{21} the exceptional divisors over the blowing up loci $\mathbb{P}_1 \times \mathbb{P}_2$ and $\mathbb{P}_2 \times \mathbb{P}_1$, respectively. Now consider the addition map $\mu : \mathcal{X}^\star \times_S \mathcal{X}^\star \to \mathcal{X}^\star$ with $\mathcal{X}^\star$ as in § 2. This morphism induces (and is induced by) a map $\tilde{\mu} : G \times_S G \to G$. However, this map does not extend to a morphism of the relatively complete model $\tilde{P}'$ since the corresponding (covariant) map $(Z^t \otimes \mathbb{R})^2 \to (Z^t \otimes \mathbb{R})$ does not map cells to cells. After subdividing (by adding the lines $x + y = l$ with $l \in \mathbb{Z}$) this property is satisfied (cf. [11], Thm. 7, p. 25). This means that the map μ extends to $\tilde{\mu} : \tilde{P}' \to \tilde{P}$ for the polyhedral decomposition given by this subdivision. It is compatible with the action of $\mathbb{Z}$ and $\mathbb{Z} \times \mathbb{Z}$ and hence descends to a morphism $\bar{\mu} : \mathcal{Y} \to \mathcal{X}$. We summarize:

Proposition 3.1. *The addition map of group schemes $\mu : \mathcal{X}^\star \times_S \mathcal{X}^\star \to X^\star$ extends to a morphism $\bar{\mu} : \mathcal{Y} \to \mathcal{X}$.*

We now describe an explicit local construction of the model $\mathcal{Y}$ by blowing up the model $\mathcal{X} \times_S \mathcal{X}$. Let $A_S^{g+1} = \operatorname{Spec}(R[x_1, \ldots, x_{g+1}])$ denote affine S-space. In local coordinates, inside A_S^{g+1}, we may assume that the g-dimensional fibration $\pi : \mathcal{X}^\star \to S$ is given by the equation $x_1 x_2 = t$, where the coordinates $x_3, \ldots, x_{g+1}$ are not involved, see [14] p. 361-362. We may assume that the zero section of the family is defined by $x_i = 1$ for $i = 1, \ldots, g+1$.
We form the fibre product $\pi : \mathcal{Y}' = \mathcal{X} \times_S \mathcal{X}$. We denote by Λ the support of the singular locus of X_0. The $(2g+1)$-dimensional variety $\mathcal{Y}'$ is singular in the special fibre along $\Sigma = \Lambda \times_k \Lambda \cong B \times_k B$ of dimension $2g-2$. The generic fibre Y'_η is the product $X_\eta \times_K X_\eta$ of the abelian variety X_η, while the zero fibre Y'_0 is singular. The local equations of $\mathcal{Y}'$ in a neighborhood of the singular locus of the family are given in our local coordinates by the system $x_1 x_2 = t$, $x'_1 x'_2 = t$. The singular locus Σ of $\mathcal{Y}'$ is given by the equations $x_1 = x_2 = x'_1 = x'_2 = t = 0$. The above blow up $\epsilon : \mathcal{Y} \to \mathcal{Y}'$ is a small blow up and can be described directly as follows: we blow up $\mathcal{Y}'$ along its subvariety Π defined by $x_1 = x'_2 = 0$ (a 2-plane contained in the central fibre of $\mathcal{Y}'$). The proper transform $\mathcal{Y}$ of $\mathcal{Y}'$ is smooth. In local coordinates, the blow-up is given by the graph $\Gamma_\phi \subseteq \mathcal{Y}' \times \mathbb{P}^1$ of the rational map $\phi : \mathcal{Y}' \longrightarrow \mathbb{P}^1$ given by $\phi(x_1, \ldots, x'_{g+1}, t) = (x_1 : x'_2)$. The equations of the graph $\Gamma_\phi \subseteq \mathcal{Y}' \times \mathbb{P}^1 \subseteq A_S^{2(g+1)} \times_S \mathbb{P}^1_S$ are given by the system

$$x_1 x_2 = t,\ u x'_2 - v x_1 = 0,\ u x_2 - v x'_1 = 0\,,$$

where u, v are homogeneous coordinates on $\mathbb{P}^1$.
For later calculations we write down the morphism $\bar{\mu}$ explicitly on the special fibre. We start with $g = 1$; then B is trivial and we may restrict the map to an irreducible component of the special fibre of the relatively complete model $\tilde{P} \times_S \tilde{P}$ and get the map $m : \mathbb{P}^1 \times \mathbb{P}^1 \to \mathbb{P}^1$ given by $((a : b), (a' : b')) \mapsto (aa' : bb')$. This is not defined in the points $(0, \infty)$ and $(\infty, 0)$. After blowing up these points (which is the blow up $\mathcal{Y} \to \mathcal{Y}'$) the rational map becomes a regular map $\tilde{m} : \tilde{V} \to \mathbb{P}^1$. It is defined by the two sections $\operatorname{prop}(p_1^*\{0\}) + \operatorname{prop}(p_2^*\{0\})$ and $\operatorname{prop}(p_1^*\{\infty\}) + \operatorname{prop}(p_2^*\{\infty\})$ of the linear system $|\tau^*(F_1 + F_2) - E_{12} - E_{21}|$ with

F_1 and F_2 the horizontal and vertical fibre (with prop( ) meaning the proper transform). The map $\tilde{m}$ descends to a map $\bar{m} : V \to \bar{\mathbb{P}}$ which is the restriction of the morphism $\bar{\mu} : \mathcal{Y} \to \mathcal{X}$ to the central fibre.
For the case $g > 1$, note that we have the addition map $\mu_{\mathcal{X}^\star}$. Its restriction to the special fibre extends to a map of the relatively complete model and then restricts to a morphism $\tilde{m} : \tilde{V} \to \mathbb{P}$ that lifts the addition map μ_B of B. That means that it comes from a surjective bundle map (cf. [10], Ch. II, Prop. 7.12)

$$\delta : m_1^*(J \oplus \mathcal{O}_B) \cong (p_1^* q^* J \otimes p_2^* q^* J) \oplus \mathcal{O}_{\tilde{V}} \to N$$

with $m_1 := \mu_B \circ (q \times q) \circ \tau : \tilde{V} \to B$ and $N = \tau^*(p_1^* \mathcal{O}(\mathbb{P}_1) \otimes p_2^* \mathcal{O}(\mathbb{P}_1)) \otimes \mathcal{O}(-E_{12} - E_{21}))$ with $p_i : \mathbb{P} \times \mathbb{P} \to \mathbb{P}$ the ith projection. Then $m_1^*(J \oplus \mathcal{O}_B)^\vee \otimes N$ is isomorphic to the direct sum of

$$\tau^* p_1^* \mathcal{O}(\mathbb{P}_i) \otimes \tau^* p_2^* \mathcal{O}(\mathbb{P}_i) \otimes \mathcal{O}(-E_{12} - E_{21}) \qquad (i = 1, 2).$$

The map δ is then given by the two sections $\mathrm{prop}(p_1^* \mathbb{P}_i) + \mathrm{prop}(p_2^* \mathbb{P}_i)$ of $\tau^* p_1^* \mathcal{O}(\mathbb{P}_i) \otimes \tau^* p_2^* \mathcal{O}(\mathbb{P}_i) \otimes \mathcal{O}(-E_{12} - E_{21})$ for $i = 1, 2$. The map $\tilde{m}$ descends to a map $\bar{m} : V \to \bar{\mathbb{P}}$ which is the restriction of the morphism $\bar{\mu} : \mathcal{Y} \to \mathcal{X}$ to the central fibre.

4. Extension of the Poincaré bundle

We denote by $j_0 : X_0 \hookrightarrow \mathcal{X}$ and $i_0 : Y_0 \hookrightarrow \mathcal{Y}$ the inclusions of the special fibre. Recall that we write V for Y_0 and $\tilde{V}$ for its normalization. We denote by $\mathcal{P}_\eta$ the Poincaré bundle on Y'_η and by P_B the Poincaré bundle on B.

Theorem 4.1. *The Poincaré bundle $\mathcal{P}_\eta$ has an extension $\mathcal{P}$ such that the pull back of $\mathcal{P}_0 := i_0^* \mathcal{P}$ to $\tilde{V}$ satisfies $\sigma^* \mathcal{P}_0 \cong \tau^*(q \times q)^* P_B \otimes \mathcal{O}(-E_{12} - E_{21})$.*

Proof. We have the following commutative diagram of maps

$$\begin{array}{ccccc}
 & & V & \xrightarrow{\bar{m}} & \bar{\mathbb{P}} \\
 & & \uparrow \sigma & & \uparrow \nu \\
 & & \tilde{V} & \xrightarrow{\tilde{m}} & \mathbb{P} \\
 & & \downarrow \tau & & \| \\
\mathbb{P} & \xleftarrow{p_i} & \mathbb{P} \times \mathbb{P} & & \mathbb{P} \\
\downarrow q & & \downarrow q \times q & & \downarrow q \\
B & \xleftarrow{q_i} & B \times B & \xrightarrow{\mu_B} & B
\end{array}$$

Let $\mathcal{L}$ be the theta line bundle on the family $\mathcal{X}$ introduced in § 2. We define the extension of $\mathcal{P}_\eta$ by

$$\mathcal{P} := \bar{\mu}^* \mathcal{L} \otimes \rho_1^* \mathcal{L}^{-1} \otimes \rho_2^* \mathcal{L}^{-1},$$

where we denote by $\rho_1, \rho_2 : \mathcal{Y} \to \mathcal{X}$ the compositions of the natural projections ${\rho'}_i : \mathcal{Y}' \to \mathcal{X}$ with the blowing up map $\epsilon : \mathcal{Y} \to \mathcal{Y}'$ of § 3. We then have $\sigma^* \mathcal{P}_0 = \sigma^*(\bar{m}^* j_0^* \mathcal{L}) \otimes \sigma^* i_0^* \rho_1^* \mathcal{L}^{-1} \otimes \sigma^* i_0^* \rho_2^* \mathcal{L}^{-1}$. Now $\bar{m}^* j_0^* \mathcal{L} = \bar{m}^* \bar{L}$ and by using the description of $\bar{L}$ in § 2 we have $\sigma^*(\bar{m}^* j_0^* \mathcal{L}) = \tilde{m}^* \nu^* \bar{L} = \tilde{m}^*(\mathcal{O}(\mathbb{P}_1) \otimes q^* M_b)$. In view of $\mathcal{O}(\mathbb{P}_1) = \mathcal{O}(1)$ we have by the discussion at the end of § 3 that

$$\tilde{m}^* \mathcal{O}(\mathbb{P}_1) = \tau^* p_1^* \mathcal{O}(\mathbb{P}_1) \otimes \tau^* p_2^* \mathcal{O}(\mathbb{P}_1) \otimes \mathcal{O}(-E_{12} - E_{21})$$

and $\tilde{m}^* q^* M_b = \tau^*(q \times q)^* \mu_B^* M_b$. On the other hand we have

$$\sigma^*(i_0^* \rho_i^* \mathcal{L}) = \tau^* p_i^* \nu^* \bar{L} = \tau^* p_i^* \mathcal{O}(\mathbb{P}_1) \otimes \tau^*(q \times q)^* q_i^* M_b$$

and putting this together we get the result. □

5. The basic construction

The fibration $\pi : \mathcal{Y} \to S$ is a flat map since $\mathcal{Y}$ is irreducible and S is smooth 1-dimensional, see [10], Ch. III, Proposition 9.7. The maps $\rho_i = \mathcal{Y} \to \mathcal{X}$, $i = 1, 2$, defined in the proof of Theorem 4.1, are flat maps too since they are maps of smooth irreducible varieties with fibres of constant dimension g, see e.g. [12], Corollary of Thm. 23.1.

We denote by Y_0 (resp. Y_η) the special fibre (resp. the generic fibre) and by $i_0 : Y_0 \to \mathcal{Y}$ (resp. $i_\eta : Y_\eta \to \mathcal{Y}$) the corresponding embedding. According to [8], Example 10.1.2, i_0 is a regular embedding. Similarly, $j_0 : X_0 \to \mathcal{X}$ is a regular embedding. We consider the diagram

$$\begin{array}{ccc} Y_0 & \xrightarrow{i_0} & \mathcal{Y} \\ \downarrow{\scriptstyle \pi_0} & & \downarrow{\scriptstyle \pi} \\ \mathrm{Spec}(k) & \xrightarrow{s} & S \end{array}$$

Let $i_0^* : A_k(\mathcal{Y}) \to A_{k-1}(Y_0)$ be the Gysin map (see [8], Example 5.2.1). Since Y_0 is an effective Cartier divisor in $\mathcal{Y}$ the Gysin map i_0^* coincides with the Gysin map for divisors (see [8], Example 5.2.1 (a) and § 2.6).

We now consider specialization of cycles, see [8], § 20.3. Note that according to [8], Remark 6.2.1., in our case we have $s^! a = i_0^* a,\ a \in A_*(\mathcal{Y})$. If $\mathcal{Z}$ is a flat scheme over the spectrum of a discrete valuation ring S the specialization homomorphism $\sigma_Z : A_k(Z_\eta) \to A_k(Z_0)$ is defined as follows, see [8], pg. 399: If β_η is a cycle on Z_η we denote by β an extension of β_η in $\mathcal{Z}$ (e.g. the Zariski closure of β_η in $\mathcal{Z}$) and then $\sigma_Z(\beta_\eta) = i_0^*(\beta)$, where $i_0 : Z_0 \to \mathcal{Z}$ is the natural embedding.

Let c_η be a cycle on X_η and let $\varphi_\eta = F(c_\eta)$ be the Fourier-Mukai transform. It is defined by $F(c_\eta) = \rho_{2*}(e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta) \in A_*(X_\eta)$. Let $\sigma_X : A_k(X_\eta) \to A_k(X_0)$ be the specialization map. We have to determine $\sigma_X(F(c_\eta))$.

If β_η is a cycle on Y_η, we have $\rho_{2*}\sigma_Y(\beta_\eta) = \sigma_X \rho_{2*}(\beta_\eta)$ by applying [8] Proposition 20.3 (a) to the proper map $\rho_2 : \mathcal{Y} \to \mathcal{X}$. By choosing $\beta_\eta = e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta$ we have

$$\sigma_X(F(c_\eta)) = \rho_{2*}\sigma_Y(e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta)\ . \tag{1}$$

Therefore, in order to compute $\sigma_X(\mathcal{F}(c_\eta))$ we have to identify $\sigma_Y(e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta)$. We take the extension $e^{c_1(\mathcal{P})}$ of $e^{c_1(\mathcal{P}_\eta)}$ and the extension of $\rho_1^* c_\eta$ given by $\rho_1^* c$,

where c is the Zariski closure of c_η in $\mathcal{X}$. Since $i_\eta : Y_\eta \to \mathcal{Y}$ is an open embedding and hence a flat map of dimension 0, we have $i_\eta^*(e^{c_1(\mathcal{P})} \cdot \rho_1^* c) = e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta$, see [8], Proposition 2.3 (d). In other words, the cycle $e^{c_1(\mathcal{P})} \cdot \rho_1^* c$ extends the cycle $e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta$ and hence $\sigma_Y(e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta) = i_0^*(e^{c_1(\mathcal{P})} \cdot \rho_1^* c)$.
Now, for any k-cycle a on $\mathcal{Y}$ we have the identity

$$i_0^*(c_1(\mathcal{P}) \cdot a) = c_1(\mathcal{P}_0) \cdot i_0^*(a)$$

in $A_{k-2}(Y_0)$, where $\mathcal{P}_0 = i_0^*\mathcal{P}$ is the pull back of the line bundle and $i_0^* a$ the Gysin pull back to the divisor Y_0. This follows from applying the formula in [8], Proposition 2.6 (e) to $i_0 : Y_0 \to \mathcal{Y}$, with $D = Y_0$, $X = \mathcal{Y}$ and $L = \mathcal{P}$ the Poincaré bundle. Hence

$$\sigma_Y(e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta) = e^{c_1(\mathcal{P}_0)} \cdot i_0^*(\rho_1^* c) \; . \tag{2}$$

By the Moving Lemma (see [8], § 11.4), we may choose the cycle c on the regular $\mathcal{X}$ such that it intersects the singular locus Λ of the central fibre properly. Since $\Lambda \subseteq X_0$ the cycle $c_0 = j_0^*(c)$ meets Λ properly by the following dimension argument. We have $\dim(c \cap \Lambda) = \dim(c_0 \cap \Lambda)$, hence

$$\begin{aligned} \dim(c_0 \cap \Lambda) &= \dim(c) + \dim(\Lambda) - \dim(X) \\ &= (\dim(c) - 1) + \dim(\Lambda) - (\dim(X) - 1) \\ &= \dim(c_0) + \dim(\Lambda) - \dim(X_0). \end{aligned}$$

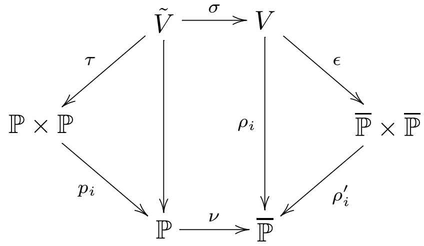
Since Λ is of codimension 1 in $X_0 = \bar{\mathbb{P}}$, saying that c_0 meets Λ properly, is equivalent to saying that no component of c_0 is contained in Λ.

Lemma 5.1. *There exists a cycle γ on $\mathbb{P}$ with $c_0 = \nu_*\gamma$ that meets the sections $\mathbb{P}_i$ for $i = 1, 2$ properly.*

Proof. If Λ is the singular locus of $\bar{\mathbb{P}}$ and $A = \mathbb{P}_1 \cup \mathbb{P}_2$ its preimage in $\mathbb{P}$, then $\bar{\mathbb{P}}\backslash\Lambda \cong \mathbb{P}\backslash A$. We may assume that the cycle c_0 is irreducible and we consider the support of $c_0 \cap (\bar{\mathbb{P}}\backslash\Lambda)$ as a subset W of $\mathbb{P}\backslash A$. Its Zariski closure $\gamma = \bar{W}$ is an irreducible cycle on $\mathbb{P}$. Then $\nu_*\gamma$ is an irreducible cycle on $\bar{\mathbb{P}}$ since the map ν is a projective map. Also, $\nu_*\gamma \cap (\bar{\mathbb{P}}\backslash\Lambda) = c_0 \cap (\bar{\mathbb{P}}\backslash\Lambda)$, hence $\nu_*\gamma$ is the Zariski closure of $c_0 \cap (\bar{\mathbb{P}}\backslash\Lambda)$ and so, by the irreducibility, we have $\nu_*\gamma = c_0$. □

Lemma 5.2. *If $c_0 = \nu_*\gamma$, then we have $i_0^*\rho_1^* c = \sigma_*(\tau^*(p_1^*\gamma))$.*

Proof. We denote the restriction of ρ_i to the special fibre again by ρ_i. Then we have $i_0^*\rho_1^* c = \rho_1^* c_0$ since ρ_1 is a flat map and i_0, j_0 are regular embeddings (see [8], Theorem 6.2 (b) and Remark 6.2.1). We will use the following commutative diagram



We may assume that c_0 and γ are irreducible k-cycles. We claim that $\rho_1^* c_0$ is irreducible. Indeed, the map ρ_1 is a flat map of relative dimension g. The cycle $\rho_1^* c_0$ is then a cycle of pure dimension $k+g$ and contains the proper transform of $(\rho_1')^* c_0$ and that is an irreducible cycle. Any other irreducible component of $\rho_1^* c_0$ must have support on the preimage of Λ. But since the cycle c_0 intersects Λ along a $k-1$-cycle, there is no irreducible component of $\rho_1^* c_0$ on the preimage of Λ. On the other hand, since γ meets the sections $\mathbb{P}_i$ properly, the cycle $\tau^* p_1^* \gamma$ is an irreducible cycle, and hence so is $\sigma_*(\tau^* p_1^* \gamma)$. But as $\rho_1^* c_0$ and $\sigma_*(\tau^* p_1^* \gamma)$ coincide outside the exceptional divisor of V, they have to coincide everywhere. □

Proposition 5.3. *We have* $\sigma_X(\mathcal{F}(c_\eta)) = \rho_{2*}(e^{c_1(\mathcal{P}_0)} \cdot \sigma_*(\tau^* p_1^* \gamma))$.

Proof. By equation (2) and Lemma 5.2 we have

$$\sigma_Y(e^{c_1(\mathcal{P}_\eta)} \cdot \rho_1^* c_\eta) = e^{c_1(\mathcal{P}_0)} \cdot \sigma_* \tau^* (p_1^* \gamma) \; . \tag{3}$$

The result follows from equation (1). □

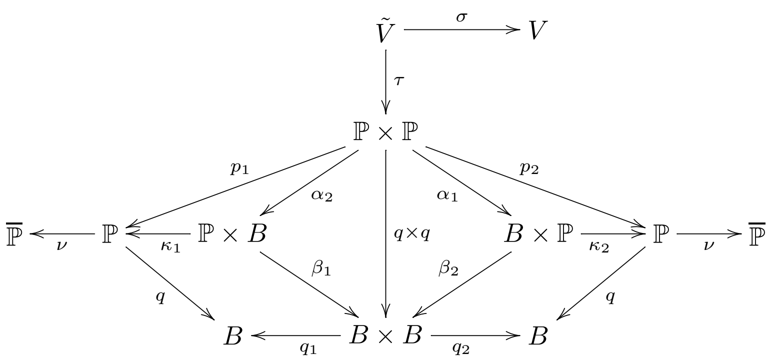
In order to calculate the limit of the Fourier-Mukai transform we are thus reduced to a calculation in the special fibre.

6. A calculation in the special fibre - Proof of the main theorem

Recall the normalization map $\sigma : \tilde{V} \to V$. Suppose we have a cycle ρ on $\tilde{V}$ with $\sigma_* \rho = c_0$. We can consider the intersection $c_1(\mathcal{P}_0)^k \cdot c_0$, that is a successive intersection of a cycle with a Cartier divisor on the singular variety V. On the other hand we have the cycle $\sigma_*(c_1(\sigma^* \mathcal{P}_0)^k \cdot \rho)$ and the projection formula ([8], Proposition 2.5 (c)) implies that

$$c_1(\mathcal{P}_0)^k \cdot c_0 = \sigma_*(c_1(\sigma^* \mathcal{P}_0)^k \cdot \rho).$$

Now we will use the following diagram of maps.



Lemma 6.1. *Let x be a cycle on $B \times B$. Then the following holds.*

(1) $p_{2*}((q \times q)^* x) = 0$.
(2) $p_{2*}((q \times q)^* x \cdot p_1^* \eta) = q^* q_{2*} x$.

Proof. For (1) we observe that $p_{2*} = \kappa_{2*}\alpha_{1*}$, and $(q \times q)^* = \alpha_1^*\beta_2^*$ and $\alpha_{1*}\alpha_1^* = 0$. For (2) we use the identities

$$\begin{aligned} p_{2*}((q \times q)^* x \cdot p_1^*\eta) &= p_{2*}(\alpha_2^*\beta_1^* x \cdot \alpha_2^*\kappa_1^*\eta) = p_{2*}\alpha_2^*(\beta_1^* x \cdot \kappa_1^*\eta) \\ &= \kappa_{2*}\alpha_{1*}\alpha_2^*(\beta_1^* x \cdot \kappa_1^*\eta) = \kappa_{2*}\beta_2^*\beta_{1*}(\beta_1^* x \cdot \kappa_1^*\eta) \\ &= \kappa_{2*}\beta_2^*(x \cdot \beta_{1*}\kappa_1^*\eta) = q^* q_{2*}(x \cdot q_1^* q_*\eta) = q^* q_{2*} x. \end{aligned}$$

□

Consider the following diagram of maps

$$\begin{array}{ccccc} \mathbb{P}_i & & \mathbb{P}_i \times \mathbb{P}_j & \xleftarrow{\pi_{ij}} & E_{ij} \\ \downarrow{\scriptstyle \lambda_i} & & \downarrow{\scriptstyle \lambda_{ij}} & & \downarrow{\scriptstyle \epsilon_{ij}} \\ \mathbb{P} & \xleftarrow{p_1} & \mathbb{P} \times \mathbb{P} & \xleftarrow{\tau} & \tilde{V} \\ \downarrow{\scriptstyle q} & & \downarrow{\scriptstyle q \times q} & & \downarrow{\scriptstyle \sigma} \\ B & \xleftarrow{q_1} & B \times B & & V \\ & & \downarrow{\scriptstyle q_2} & & \\ & & B & & \end{array}$$

where p_i, q_i are the projections to the ith factor, π_{ij} the canonical map of the projective bundle E_{ij} and the maps λ_i, λ_{ij} and ϵ_{ij} the natural inclusions. The map $(q \times q) \circ \lambda_{ij}$ is an isomorphism.
By the adjunction formula, the normal bundles to $\mathbb{P}_1$, $\mathbb{P}_2$ are $N_{\mathbb{P}_1}(\mathbb{P}) = J$ and $N_{\mathbb{P}_2}(\mathbb{P}) = J^{-1}$. The exceptional divisors E_{12} and E_{21} are projective bundles over the blowing up loci $\mathbb{P}_i \times \mathbb{P}_j$. By identifying $\mathbb{P}_i \times \mathbb{P}_j$ with $B \times B$, via the map $(q \times q) \circ \lambda_{ij}$, we have $E_{12} = \mathbb{P}(q_1^* J^{-1} \oplus q_2^* J)$ and $E_{21} = \mathbb{P}(q_1^* J \oplus q_2^* J^{-1})$. We set $\xi_{ij} = c_1(O(1))$ on E_{ij}. By standard theory [[10], ch. II, Theorem 8.24 (c)] we have $\epsilon_{ij}^* E_{ij} = -\xi_{ij}$.
We now introduce the notation

$$\gamma := c_1(J), \quad \gamma_i = q_i^*\gamma, \quad \eta_i = p_i^*\eta, \quad i = 1, 2.$$

Note that γ is algebraically equivalent to 0, but not rationally equivalent to 0. We have the quadratic relations

$$(\xi_{ij} - {\pi'_{ij}}^*\gamma_j)(\xi_{ij} + {\pi'_{ij}}^*\gamma_i) = 0$$

where $\pi'_{ij} : E_{ij} \to B \times B$ is the natural map, showing that ξ_{ij}^2 is expressible in lower powers.

Lemma 6.2. *Suppose that ξ satisfies the relation $\xi^2 + (a - b)\xi - ab = 0$. Then, with $\phi_k = (b^k - (-a)^k)/(b + a)$ we have $\xi^k = \phi_k\xi + ab\phi_{k-1}$ for any $k \geq 1$ (where we put $\phi_0 = 0$).*

Proof. Immediate by checking the relation with $\xi = b$ or $\xi = -a$. □

Applying the above for the classes ξ_{ij} of the bundles E_{ij}, considered as bundles over $B \times B$ via the isomorphism $(q \times q) \circ \lambda_{ij}$, we get, by choosing

$$\phi_k = \sum_{m=0}^{k-1} (-1)^m \gamma_1^m \gamma_2^{k-1-m},$$

that

$$\begin{aligned} \xi_{12}^k =& {\pi'}_{12}^{*} \phi_k \cdot \xi_{12} + {\pi'}_{12}^{*} (\gamma_1 \gamma_2 \phi_{k-1}), \\ \xi_{21}^k =& (-1)^{k+1} {\pi'}_{21}^{*} \phi_k \cdot \xi_{21} + (-1)^k {\pi'}_{21}^{*} (\gamma_1 \gamma_2 \phi_{k-1}). \end{aligned}$$

We view now the bundles E_{ij} as bundles over $\mathbb{P}_i \times \mathbb{P}_j$ and, for any $k \geq 0$, we write $\xi_{ij}^k = \pi_{ij}^* A_{ij}(k) \xi_{ij} + \pi_{ij}^* B_{ij}(k)$, for some cycles $A_{ij}(k)$, $B_{ij}(k)$ on $\mathbb{P}_i \times \mathbb{P}_j$. By the above relations we have

$$(q \times q)_* \lambda_{ij*} A_{ij}(k) = (-1)^{(k+1)j} \phi_k .$$

Lemma 6.3. *We have*

$$\lambda_{ij*} A_{ij}(k) = (-1)^{(k+1)j} [(q \times q)^* \phi_k \cdot \eta_1 \eta_2 - (q \times q)^* (\phi_k \, \gamma_j) \cdot \eta_i] .$$

Proof. We let $\psi_{ij} = (q \times q) \circ \lambda_{ij} : \mathbb{P}_i \times \mathbb{P}_j \to B \times B$ be the natural isomorphism. We then have the identity

$$\lambda_{ij*} A_{ij}(k) = \lambda_{ij*}(\psi_{ij}^* \psi_{ij*} A_{ij}(k)) = (q \times q)^* \psi_{ij*} A_{ij}(k) \cdot \lambda_{ij*} 1_{\mathbb{P}_i \times \mathbb{P}_j}.$$

But $\lambda_{ij*} 1_{\mathbb{P}_i \times \mathbb{P}_j} = p_1^* \mathbb{P}_i \cdot p_2^* \mathbb{P}_j = \eta_i (\eta_j - p_j^* q^* \gamma) = \eta_1 \eta_2 - \eta_i \cdot (q \times q)^* \gamma_j$ and the result follows. □

Lemma 6.4. *For a cycle class $x = q^* z + q^* w \cdot \eta$ on $\mathbb{P}$ the cycle class $\tau_*(\tau^* p_1^* x \cdot (E_{12}^k + E_{21}^k))$ for $k \geq 1$ is given by*

$$\begin{aligned} &\sum_{m=0}^{k-2} (-1)^m \{ (q \times q)^* q_1^* [(((-1)^{k+1} - 1) z + (-1)^{k+1} w \gamma) \, \gamma^m] \cdot \eta_1 \eta_2 \\ &+ (-1)^k (q \times q)^* q_1^* [(z + w\gamma) \, \gamma^m] \cdot \eta_1 \cdot p_2^* q^* \gamma \\ &+ (q \times q)^* q_1^* (z \gamma^{m+1}) \cdot \eta_2 \} \cdot p_2^* q^* \gamma^{k-2-m}. \end{aligned}$$

Note that for $k = 1$ the above sum is zero.

Proof. Since $\epsilon_{ij}^* E_{ij} = -\xi_{ij}$ we have $E_{ij}^k = (-1)^{k-1} \epsilon_{ij*} \xi_{ij}^{k-1}$. Therefore

$$\begin{aligned} \tau_*(\tau^* p_1^* x \cdot E_{ij}^k) =& (-1)^{k-1} p_1^* x \cdot \tau_* \epsilon_{ij*} \xi_{ij}^{k-1} \\ =& (-1)^{k-1} p_1^* x \cdot \lambda_{ij*} \pi_{ij*} (\pi_{ij}^* A_{ij}(k-1) \xi_{ij} + \pi_{ij}^* B_{ij}(k-1)) \\ =& (-1)^{k-1} p_1^* x \cdot \lambda_{ij*} A_{ij}(k-1) \end{aligned}$$

since $\pi_{ij*} \xi_{ij} = 1_{\mathbb{P}_i \times \mathbb{P}_j}$. Note that since $A_{ij}(0) = 0$ the above calculation shows that $\tau_*(\tau^* p_1^* x \cdot E_{ij}) = 0$. By Lemma 6.3 and by using the relation

$$p_1^* x = (q \times q)^* q_1^* z + (q \times q)^* q_1^* w \cdot \eta_1,$$

we have

$$\begin{aligned} \tau_*(\tau^* p_1^* x \cdot E_{ij}^k) =& (-1)^{k(j+1)+1} ((q \times q)^* q_1^* z + (q \times q)^* q_1^* w \cdot \eta_1) \\ & \cdot [(q \times q)^* \phi_{k-1} \cdot \eta_1 \eta_2 - (q \times q)^* (\phi_{k-1} \gamma_j) \cdot \eta_i] \end{aligned}$$

and this equals

$$(-1)^{k(j+1)+1}[(q\times q)^*(q_1^*z\cdot\phi_{k-1})\cdot\eta_1\eta_2-(q\times q)^*(q_1^*z\cdot\phi_{k-1}\gamma_j)\cdot\eta_i$$
$$+(q\times q)^*(q_1^*w\cdot\phi_{k-1})\cdot\eta_1^2\eta_2-(q\times q)^*(q_1^*w\cdot\phi_{k-1}\gamma_j)\cdot\eta_1\eta_i]$$

We then have, by using the formula $\eta^2=q^*\gamma\cdot\eta$, that

$$\tau_*(\tau^*p_1^*x\cdot E_{12}^k)=(-1)^{k+1}[(q\times q)^*(q_1^*(z+w\gamma)\cdot\phi_{k-1})\cdot\eta_1\eta_2$$
$$-(q\times q)^*(q_1^*(z+w\gamma)\cdot\phi_{k-1})\cdot\eta_1\cdot p_2^*q^*\gamma]$$

and

$$\tau_*(\tau^*p_1^*x\cdot E_{21}^k)=-(q\times q)^*(q_1^*z\cdot\phi_{k-1})\cdot\eta_1\eta_2+(q\times q)^*(q_1^*(z\,\gamma)\cdot\phi_{k-1})\cdot\eta_2.$$

Using $\phi_{k-1}=\sum_{m=0}^{k-2}(-1)^m\gamma_1^m\cdot\gamma_2^{k-2-m}$ we deduce the proposition. □

We state now the basic result of this section.

Proposition 6.5. *Let z, w be cycles on B. Then we have*

$$p_{2*}\tau_*(e^{c_1(\sigma^*\mathcal{P}_0)}\cdot\tau^*(p_1^*(q^*z+q^*w\cdot\eta))=q^*a+q^*b\cdot\eta,$$

with a and b as in Theorem 1.1.

Proof. We put $x=q^*z+q^*w\cdot\eta$. We want to calculate

$$p_{2*}\tau_*(e^{\tau^*(q\times q)^*c_1(P_B)-E_{12}-E_{21}}\cdot\tau^*(p_1^*x))$$

which equals

$$p_{2*}(e^{(q\times q)^*c_1(P_B)}\cdot\tau_*(e^{-E_{12}-E_{21}}\cdot\tau^*p_1^*x)).$$

Since $E_{12}\cdot E_{21}=0$ we have

$$e^{-E_{12}-E_{21}}=1+\sum_{k=1}^{2g}\frac{(-1)^k}{k!}\,(E_{12}^k+E_{21}^k)$$

and so $\tau_*(e^{-E_{12}-E_{21}}\cdot\tau^*p_1^*x)$ equals

$$p_1^*x+\sum_{k=1}^{2g}\frac{(-1)^k}{k!}\,\tau_*[\tau^*p_1^*x\cdot(E_{12}^k+E_{21}^k)].$$

We have

$$p_{2*}((q\times q)^*e^{c_1(P_B)}\cdot p_1^*x)=$$
$$=p_{2*}(e^{(q\times q)^*c_1(P_B)}\cdot p_1^*(q^*z+q^*w\,\eta))$$
$$=p_{2*}((q\times q)^*(e^{c_1(P_B)}q_1^*z)+(q\times q)^*(e^{c_1(P_B)}q_1^*w)\,p_1^*\eta)$$
$$=0+q^*q_{2*}(e^{c_1(P_B)}q_1^*w)=q^*F_B(w)$$

by Lemma 6.1. Combining the above with Lemma 6.4 we find that

$$p_{2*}\tau_*(e^{\tau^*(q\times q)^*c_1(P_B)-E_{12}-E_{21}}\cdot\tau^*(p_1^*x))$$

is the sum of the four terms: the first is $q^*F_B(w)$, the second is

$$\sum_{k=2}^{2g}\sum_{m=0}^{k-2}\frac{(-1)^{k+m}}{k!}\{p_{2*}[(q\times q)^*[e^{c_1(P_B)}q_1^*[(((-1)^{k+1}-1)z+ (-1)^{k+1}w\gamma)\,\gamma^m]]\cdot\eta_1]\}\cdot\eta\cdot q^*\gamma^{k-2-m},$$

the third term is

$$\sum_{k=2}^{2g}\sum_{m=0}^{k-2}\frac{(-1)^{m}}{k!}\{p_{2*}[(q\times q)^*[e^{c_1(P_B)}q_1^*[(z+w\gamma)\,\gamma^m]]\cdot\eta_1]\}\cdot q^*\gamma^{k-1-m},$$

and finally the fourth is

$$\sum_{k=2}^{2g}\sum_{m=0}^{k-2}\frac{(-1)^{k+m}}{k!}\{p_{2*}[(q\times q)^*[e^{c_1(P_B)}q_1^*(z\gamma^{m+1})]]\}\cdot\eta\cdot q^*\gamma^{k-2-m}\,.$$

By applying now Lemma 6.1 and by making the substitution $n=k-2$ we get the desired expression. □

Corollary 6.6. *Let z, w be cycles on B. Then modulo algebraic equivalence we have*

$$p_{2*}\tau_*(e^{c_1(\sigma^*\mathcal{P}_0)}\cdot\tau^*(p_1^*(q^*z+q^*w\cdot\eta))\overset{a}{=}q^*F_B(w)-q^*F_B(z)\cdot\eta.$$

Proof. Indeed, since $c_1(J)\overset{a}{=}0$ it is clear that $a\overset{a}{=}F_B(w)$ and $b\overset{a}{=}-q^*F_B(z)$ since the only non zero term of the sum corresponds to $m=0,\ n=0$. □

We conclude now with the proof of the basic Theorem 1.1 and Theorem 1.2:

Proof. By Proposition 5.3 we have $\varphi_0=\sigma_X F(c_\eta)=\rho_{2*}(e^{c_1(\mathcal{P}_0)}\cdot\sigma_*(\tau^*p_1^*\gamma))$. By the projection formula we have $e^{c_1(\mathcal{P}_0)}\cdot\sigma_*(\tau^*p_1^*\gamma)=\sigma_*(e^{c_1(\sigma^*\mathcal{P}_0)}\cdot\tau^*p_1^*\gamma)$. Observe now that $\rho_2\circ\sigma=\nu\circ(p_2\circ\tau):\tilde{V}\to\bar{\mathbb{P}}$, see the diagram in the proof of Lemma 5.2. The proof then follows from Proposition 6.5 and Corollary 6.6. □

7. Applications

Let $\mathcal{X}\to S$ be a completed rank-one degeneration as described in § 2. According to Beauville [2] we have a decomposition of $A^i_{\mathbb{Q}}(X_\eta)$ into subspaces which are eigenspaces for the action by multiplication by an integer on X_η:

$$A^i_{\mathbb{Q}}(X_\eta)=\oplus_j A^i_{(j)}(X_\eta)$$

such that $n^*(x)=n^{2i-j}\,x$ for $x\in A^i(X_\eta)$. (Beauville works over $\mathbb{C}$, but his proof does not use more than the Fourier-Mukai transform which works over the residue field of η.) The multiplication map n acts as multiplication by n^{2i} on homology and therefore all cycles in $A^i_{(j)}(X_\eta)$ are homologically trivial for $j\neq 0$. Since under the Fourier-Mukai transform we have $F(A^i_{(j)}(X_\eta))=A^{g-i+j}_{(j)}(X_\eta)$, the elements of A^i that lie in $A^i_{(j)}$ are characterized by the codimension of their Fourier transform (namely $g-i+j$).

Suppose now that $c = \sum c^{(j)} \in A^i(X_\eta)$ with $c^{(j)} \in A^i_{(j)}(X_\eta)$, where the decomposition corresponds to $\varphi := F(c) = \sum \varphi^{(j)}$ with $\varphi^{(j)} \in A^{g-i+j}(X_\eta)$.

Theorem 7.1. *Let $c = c_\eta = \sum c^{(j)} \in A^i(X_\eta)$ with $c^{(j)} \in A^i_{(j)}(X_\eta)$. Assume for some j' that $\varphi_0^{(j')} \neq 0$, where φ_0 is the specialization of φ and $\varphi_0^{(j')}$ the codimension $g-i+j'$-part of φ_0. Then $c^{(j')} \neq 0$.*

Proof. The specialization map preserves the codimension of cycles. Therefore, if $c^{(j')} = 0$ then $\varphi^{(j')} = 0$, hence $\varphi_0^{(j')} = 0$ and this contradicts our assumption. □

This theorem, which holds as well for cycles modulo algebraic equivalence, can be used to prove non-vanishing results for cycles. For the rest of this section we work modulo algebraic equivalence. For example, consider a threefold $\mathcal{Z}/S$ such that Z_η is a smooth cubic threefold and Z_0 is a generic nodal cubic threefold. We shall consider the Picard variety of the Fano surface of this degenerating cubic threefold and this will give us a degenerating abelian variety of dimension 5, cf. [5].

As is well-known the nodal cubic threefold Z_0, and hence its Fano surface, corresponds to a canonical genus 4 curve C in $\mathbb{P}^3$, see e.g. [9] Section 2. The genericity assumption means that the curve C is a generic curve and hence we may assume by Ceresa's result [4] that the class $C^{(1)}$ does not vanish in the Jacobian B of the curve C. Since C is a trigonal curve we have by [6] that $C^{(j)} \overset{a}{=} 0$ for $j \geq 2$. Hence the Beauville decomposition of C is $[C] \overset{a}{=} C^{(0)} + C^{(1)}$ with $F_B(C^{(0)}) \in A^1_{(0)}(B)$ and $F_B(C^{(1)}) \in A^2_{(1)}(B)$.

The Picard variety $\mathcal{X}/S$ of the Fano surface of $\mathcal{Z}/S$ defines a principally polarized semi-abelian variety with central fibre a rank-one extension of the Jacobian B of the curve C, see [9], Corollary 6.3 and Section 10. The principal polarization on X_η is induced by a geometrically defined divisor Θ. Let Σ be the Fano surface of lines in Z_η. If $s \in \Sigma$ we denote by l_s the corresponding line in Z_η. For each $s \in \Sigma$ we have the divisor

$$D_s = \{s' \in \Sigma,\ l_{s'} \cap l_s \neq \emptyset\}$$

on Σ as defined in [5]. We then have a natural map

$$\Sigma \to \mathrm{Pic}^0(\Sigma), \qquad s \mapsto D_s - D_{s_0},$$

with $s_0 \in \Sigma$ a base point. It is well known that the cohomology class of Σ in $\mathrm{Pic}^0(\Sigma)$ is equal to that of the cycle $\Theta^3/3!$, see [5]. By [2], Propositions 3 and 4, we have that $A^3_{(j)}(X_\eta) = 0$ for $j < 0$ and $A^5_{(j)}(X_\eta) = 0$ for $j \neq 0$. We have therefore the decomposition

$$[\Sigma] \overset{a}{=} \Sigma^{(0)} + \Sigma^{(1)} + \Sigma^{(2)} \qquad \text{with } \Sigma^{(j)} \in A^3_{(j)}.$$

Indeed, $\Sigma^{(j)} \in A^3_{(j)}(X_\eta)$, hence $F(\Sigma^{(j)}) \in A^{2+j}_{(j)}(X_\eta)$ which is zero for $j \geq 3$. Now we show that $\Sigma^{(1)} \overset{a}{\neq} 0$, and we thus obtain a cycle which is homologically

but not algebraically equivalent to zero. Since $\Theta \in A^1_{(0)}(X_\eta)$ this implies that Σ is homologically, but not algebraically equivalent to $\Theta^3/3!$.
We denote by $\mathcal{X}$ the completed rank one degeneration of X_η. The class $[\Sigma]$ degenerates to a cycle $[\Sigma_0] = \nu_*(\gamma)$ on the central fibre X_0 of class

$$\gamma \overset{a}{=} q^*[C] + \frac{1}{2}\, q^*[C * C] \cdot \eta,$$

where $C * C$ is the Pontryagin product, see [9], Propositions 10.1 and 8.1. In order to see that $\Sigma^{(1)} \overset{a}{\neq} 0$ it suffices by Theorem 7.1 to show that $\varphi_0^{(1)} \overset{a}{\neq} 0$ with φ_0 the limit of the Fourier-Mukai transform. By Theorem 1.2, we have

$$\varphi_0 \overset{a}{=} \nu_*(\frac{1}{2}\, q^*[F_B(C) \cdot F_B(C)] - q^* F_B(C) \cdot \eta),$$

hence

$$\varphi_0^{(1)} \overset{a}{=} \nu_*(q^*[F_B(C^{(0)}) \cdot F_B(C^{(1)})] - q^* F_B(C^{(1)}) \cdot \eta).$$

Since $C^{(1)} \overset{a}{\neq} 0$ we conclude that $\varphi_0^{(1)} \overset{a}{\neq} 0$, and this implies the result.
By using the specialization of the Fourier-Mukai transform we can deduce the specialization of the Beauville decomposition. We do this working modulo algebraic equivalence.

Proposition 7.2. *Let $c = c_\eta \in A^i(X_\eta)$ with specialization $c_0 = \nu_*(q^*z + q^*w \cdot \eta)$, where $z \in A^i(B)$ and $w \in A^{i-1}(B)$. Let $c = \sum c^{(j)}$ with $c^{(j)} \in A^i_{(j)}(X_\eta)$, and let $z = \sum z^{(j)}$ with $z^{(j)} \in A^i_{(j)}(B)$ and $w = \sum w^{(j)}$ with $w^{(j)} \in A^{i-1}_{(j)}(B)$ be the Beauville decompositions. If $c_0^{(j)}$ is the specialization of $c^{(j)}$, then*

$$c_0^{(j)} \overset{a}{=} \nu_*(q^* z^{(j)} + q^* w^{(j)} \cdot \eta)\,.$$

Proof. By the proof of the main theorem in [2], the component $c^{(j)}$ is defined as $(-1)^g F((-1)^* \phi^{(j)})$ with $\phi^{(j)} \in A^{g-i+j}(X_\eta)$ (notation as above). The inversion on X_η leaves the cell decomposition of the toroidal compactification invariant and hence extends naturally to X_0. So $c_0^{(j)}$ equals $(-1)^g F((-1)^* \phi_0^{(j)})$ with $\phi_0^{(j)} \in A^{g-i+j}(X_0)$. Therefore, by Theorem 1.2, we have

$$\begin{aligned} c_0^{(j)} &\overset{a}{=} (-1)^g F((-1)^* \nu_*(q^* F_B(w^{(j)}) - q^* F_B(z^{(j)}) \cdot \eta)) \\ &\overset{a}{=} (-1)^{g+j} (-1)^{g-1+j} \nu_*(-q^* z^{(j)} - q^* w^{(j)} \cdot \eta) = \nu_*(q^* z^{(j)} + q^* w^{(j)} \cdot \eta)\,. \end{aligned}$$

□

For example, let $\mathcal{C} \to S$ be a genus g curve with C_η a smooth curve and C_0 a one-nodal curve with normalization $\tilde{C}_0$. Let p be the node of C_0 and $x_1,\ x_2$ the points of $\tilde{C}_0$ lying over p. The compactified Jacobian $\mathcal{X} = \overline{P_{\mathcal{C}/S}}$ is then a complete rank one degeneration with central fibre the $\mathbb{P}^1$-bundle over $\mathrm{Pic}^0(\tilde{C}_0)$ associated to the line bundle $J = O(x_1 - x_2)$. Let $\bar{u} : \mathcal{C} \to \mathcal{X}$ be the compactified Abel-Jacobi map and let $c_\eta = [\bar{u}(C_\eta)]$. The cycle c_η specializes then to the cycle $c_0 = [\bar{u}(C_0)]$ with $c_0 \overset{a}{=} \nu_*(q^*[\mathrm{pt}] + q^* \tilde{c}_0 \cdot \eta)$, where [pt] is the class of a point and $\tilde{c}_0$ is the class of the Abel-Jacobi image of the smooth curve $\tilde{C}_0$ in $\mathrm{Pic}^0(\tilde{C}_0)$, see e.g. [9], Proposition 7.1. By Proposition 7.2 we have then

$$c_0^{(j)} \stackrel{a}{=} \begin{cases} q^*\tilde{c}_0^{(j)} \cdot \eta, & j \neq 0\,, \\ q^*[\mathrm{pt}] + q^*\tilde{c}_0^{(0)} \cdot \eta, & j = 0\,. \end{cases}$$

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An Inverse K-Theory Functor

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Abstract. Thomason showed that the K-theory of symmetric monoidal categories models all connective spectra. This paper describes a new construction of a permutative category from a Γ-space, which is then used to re-prove Thomason's theorem and a non-completed variant.

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1. Introduction

In [15], Segal described a functor from (small) symmetric monoidal categories to infinite loop spaces, or equivalently, connective spectra. This functor is often called the K-theory functor: When applied to the symmetric monoidal category of finite rank projective modules over a ring R, the resulting spectrum is Quillen's algebraic K-theory of R. A natural question is then which connective spectra arise as the K-theory of symmetric monoidal categories? Thomason answered this question in [18], showing that every connective spectrum is the K-theory of a symmetric monoidal category; moreover, he showed that the K-theory functor is an equivalence between an appropriately defined stable homotopy category of symmetric monoidal categories and the stable homotopy category of connective spectra.

This paper provides a new proof of Thomason's theorem by constructing a new homotopy inverse to Segal's K-theory functor. As a model for the category of infinite loop spaces, we work with Γ-spaces, following the usual conventions of [1, 4]: We understand a Γ-space to be a functor X from Γ^{op} (finite based sets) to based simplicial sets such that $X(\mathbf{0}) = *$. A Γ-space has an associated spectrum [15, §1] (or [4, §4] with these conventions), and a map of Γ-spaces $X \to Y$ is called a *stable equivalence* when it induces a stable equivalence of

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the associated spectra. We understand the stable homotopy category of Γ-spaces to be the homotopy category obtained by formally inverting the stable equivalences. The foundational theorem of Segal [15, 3.4], [4, 5.8] is that the stable homotopy category of Γ-spaces is equivalent to the stable category of connective spectra.

On the other side, the category of small symmetric monoidal categories admits a number of variants, all of which have equivalent stable homotopy categories. We discuss some of these variants in Section 3 below. For definiteness, we state the main theorem in terms of the category of small permutative categories and strict maps: The objects are the small permutative categories, i.e., those symmetric monoidal categories with strictly associative and unital product, and the maps are the functors that strictly preserve the product, unit, and symmetry. Segal [15, §2] constructed K-theory as a composite functor $K' = N \circ \mathcal{K}'$ from permutative categories to Γ-spaces, where $\mathcal{K}'$ is a functor from permutative categories to Γ-categories, and N is the nerve construction applied objectwise to a Γ-category to obtain a Γ-space. We actually use a slightly different but weakly equivalent functor $K = N \circ \mathcal{K}$ described in Section 3. A *stable equivalence* of permutative categories is defined to be a map that induces a stable equivalence on K-theory Γ-spaces. (We review an equivalent more intrinsic homological definition of stable equivalence in Proposition 3.8 below.) We understand the stable homotopy category of small permutative categories to be the homotopy category obtained from the category of small permutative categories by formally inverting the stable equivalences.

In Section 4, we construct a functor P from Γ-spaces to small permutative categories. Like K, we construct P as a composite functor $P = \mathcal{P} \circ \mathcal{S}$, with $\mathcal{P}$ a functor from Γ-categories to permutative categories and $\mathcal{S}$ a functor from simplicial sets to categories applied objectwise. The functor $\mathcal{S}$ is the left adjoint of the Quillen equivalence between the category of small categories and the category of simplicial sets from [7, 17]; the right adjoint is $\mathrm{Ex}^2 N$, where Ex is Kan's right adjoint to the subdivision functor Sd. As we review in Section 2, we have natural transformations

$$(1.1) \qquad N\,\mathcal{S}\,X \longleftarrow \mathrm{Sd}^2 X \longrightarrow X \qquad \text{and} \qquad \mathcal{S}\,N\mathcal{X} \longrightarrow \mathcal{X}$$

which are always weak equivalences, where we understand a weak equivalence of categories as a functor that induces a weak equivalences on nerves. The functor $\mathcal{P}$ from Γ-categories to permutative categories is a certain Grothendieck construction (homotopy colimit)

$$\mathcal{P}(\mathcal{X}) = \mathcal{A} \textstyle\int A\mathcal{X},$$

we describe in detail in Section 4. In brief, $\mathcal{A}$ is a category whose objects are the sequences of positive integers $\vec{m} = (m_1, \ldots, m_r)$ including the empty sequence, and whose morphisms are generated by permuting the sequence, maps of finite (unbased) sets, and partitioning; for a Γ-category X, we get a (strict) functor $A\mathcal{X}$ from $\mathcal{A}$ to the category of small categories satisfying

$$A\mathcal{X}(m_1, \ldots, m_r) = \mathcal{X}(\mathbf{m}_1) \times \cdots \times \mathcal{X}(\mathbf{m}_r)$$

and $A\mathcal{X}() = \mathcal{X}(\mathbf{0}) = *$ (the category with a unique object $*$ and unique morphism). The concatenation of sequences induces the permutative product on $\mathcal{P}\mathcal{X}$ with $*$ in $A\mathcal{X}()$ as the unit. In Section 4, we construct a natural transformation of permutative categories and natural transformations of Γ-categories

$$\mathcal{P}\mathcal{K}\mathcal{C} \longrightarrow \mathcal{C} \qquad \text{and} \qquad \mathcal{X} \longleftarrow \mathcal{W}\mathcal{X} \longrightarrow \mathcal{K}\mathcal{P}\mathcal{X}, \tag{1.2}$$

where $\mathcal{W}$ is a certain functor from Γ-categories to itself (Definition 4.8). In Section 5, we show that these natural transformations are natural stable equivalences, which then proves the following theorem, the main theorem of the paper.

Theorem 1.3. *The functor P from Γ-spaces to small permutative categories preserves stable equivalences. It induces an equivalence between the stable homotopy category of Γ-spaces and the stable homotopy category of permutative categories, inverse to Segal's K-theory functor.*

The arguments actually prove a "non-group-completed" version of this theorem. To explain this, recall that a Γ-space X is called *special* [4, p. 95] when the canonical map $X(\mathbf{a} \vee \mathbf{b}) \to X(\mathbf{a}) \times X(\mathbf{b})$ is a weak equivalence for any finite based sets $\mathbf{a}$ and $\mathbf{b}$; we define a special Γ-category analogously. Note that because of the weak equivalences in (1.1), a Γ-category $\mathcal{X}$ is special if and only if the Γ-space $N\mathcal{X}$ is special, and a Γ-space X is special if and only if the Γ-category $\mathcal{S}X$ is special. For special Γ-spaces, the associated spectrum is an Ω-spectrum after the zeroth space [15, 1.4]; the associated infinite loop space is the group completion of $X(\mathbf{1})$. For any permutative category $\mathcal{C}$, $K\mathcal{C}$ is a special Γ-space and $\mathcal{K}\mathcal{C}$ is a special Γ-category. We show in Corollary 5.5 that the natural transformation $\mathcal{P}\mathcal{K}\mathcal{C} \to \mathcal{C}$ of (1.2) is a weak equivalence for any permutative category $\mathcal{C}$, and we show in Theorem 4.10 and Corollary 5.6 that the natural transformations $W\mathcal{X} \to \mathcal{X}$ and $W\mathcal{X} \to \mathcal{K}\mathcal{P}\mathcal{X}$ of (1.2) are (objectwise) weak equivalences for any special Γ-category $\mathcal{X}$. We obtain the following theorem.

Theorem 1.4. *The following homotopy categories are equivalent:*

(i) *The homotopy category obtained from the category of small permutative categories by inverting the weak equivalences.*
(ii) *The homotopy category obtained from the subcategory of special Γ-spaces by inverting the objectwise weak equivalences.*

Theorem 1.3 implies that for an arbitrary Γ-space X, the Γ-space KPX is a special Γ-space stably equivalent to X. A construction analogous to $\mathcal{P}$ on the simplicial set level produces such a special Γ-space more directly: For a Γ-space X, we get a functor AX from $\mathcal{A}$ to based simplicial sets with

$$AX(m_1, \ldots, m_r) = X(\mathbf{m}_1) \times \cdots \times X(\mathbf{m}_r)$$

and $AX() = X(\mathbf{0}) = *$. Define

$$EX = \operatorname{hocolim}_{\mathcal{A}} AX.$$

Using the Γ-spaces $X(\mathbf{n} \wedge (-))$, we obtain a Γ-space $E^\Gamma X$,

$$E^\Gamma X(\mathbf{n}) = E(X(\mathbf{n} \wedge (-)))/N\mathcal{A},$$

with $EX \to E^\Gamma X(\mathbf{1})$ a weak equivalence. The inclusion of $X(\mathbf{1})$ as $AX(1)$ provides a natural transformation of simplicial sets $X(\mathbf{1}) \to EX$ and of Γ-spaces $X \to E^\Gamma X$. In Section 6, we prove the following theorems about these constructions.

Theorem 1.5. *For any* Γ*-space* X*, the* Γ*-space* $E^\Gamma X$ *is special and the natural map* $X \to E^\Gamma X$ *is a stable equivalence. If* X *is special, then the natural map* $X \to E^\Gamma X$ *is an objectwise weak equivalence.*

Theorem 1.6. *For any* Γ*-space* X*, the simplicial set* EX *has the natural structure of an* E_∞ *space over the Barratt-Eccles operad (and in particular the structure of a monoid).*

The previous two theorems functorially produce two additional infinite loop spaces from the Γ-space X, the infinite loop space of the spectrum associated to $E^\Gamma X$ and the group completion of EX. Since the map $X \to E^\Gamma X$ is a stable equivalence, it induces a stable equivalence of the associated spectra and hence the associated infinite loop spaces. The celebrated theorem of May and Thomason [12] then identifies the group completion of EX.

Corollary 1.7. *For any* Γ*-space* X*, the group completion of the* E_∞ *space* EX *is equivalent to the infinite loop space associated to* X*.*

As a consequence of Theorem 1.5, the Γ-space $E^\Gamma X$ is homotopy initial among maps from X to a special Γ-space. Theorem 1.6 then identifies $EX \simeq E^\Gamma X(\mathbf{1})$ as a reasonable candidate for the (non-completed) E_∞ space of X. Motivated by Theorem 1.4, we propose the following definition.

Definition 1.8. We say a map of Γ-spaces $X \to Y$ is a *pre-stable equivalence* when the map $EX \to EY$ is a weak equivalence.

With this definition we obtain the equivalence of the last three homotopy categories in the following theorem from the theorems above. We have included the first category for easy comparison with other non-completed theories of E_∞ spaces; we prove the equivalence in Section 6.

Theorem 1.9. *The following homotopy categories are equivalent:*

(i) *The homotopy category obtained from the category of* E_∞ *spaces over the Barratt-Eccles operad (in simplicial sets) by inverting the weak equivalences.*
(ii) *The homotopy category obtained from the category of* Γ*-spaces by inverting the pre-stable equivalences.*
(iii) *The homotopy category obtained from the subcategory of special* Γ*-spaces by inverting the objectwise weak equivalences.*
(iv) *The homotopy category obtained from the category of small permutative categories by inverting the weak equivalences.*

The previous theorem provides a homotopy theory for permutative categories and Γ-spaces before group completion, which now allows the construction of "spectral monoid rings" associated to Γ-spaces. For a topological monoid M, the suspension spectrum $\Sigma^{\infty}_{+}M$ has the structure of an associative S-algebra (A_{∞} ring spectrum) with M providing the multiplicative structure. The spectral monoid ring is a stable homotopy theory refinement of the monoid ring $\mathbb{Z}[\pi_0 M]$, which is $\pi_0\Sigma^{\infty}_{+}M$ or $\pi_0^S M$. For a Γ-space X, we can use EX in place of M and $\Sigma^{\infty}_{+}EX$ is an E_{∞} ring spectrum with the addition on EX providing the multiplication on $\Sigma^{\infty}_{+}EX$. The spectral group ring of the associated infinite loop space, $\Sigma^{\infty}_{+}\Omega^{\infty}X$, is the localization of $\Sigma^{\infty}_{+}EX$ with respect the multiplicative monoid $\pi_0 EX \subset \pi_0^S EX$. Spectral monoid rings and algebras arise in the construction of twisted generalized cohomology theories (as explained, for example, in [3, 2.5] and [2]), and the localization $\Sigma^{\infty}_{+}EX \to \Sigma^{\infty}_{+}\Omega^{\infty}X$, specifically, plays a role in current work in extending notions of log geometry to derived algebraic geometry and stable homotopy theory (see the lecture notes by Rognes on log geometry available at [14]).

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2. Review of Γ-categories and Γ-spaces

This section briefly reviews the equivalence between the homotopy theory of Γ-spaces and of Γ-categories. We begin by introducing the notation used throughout the paper.

Notation 2.1. We denote by $\underline{n}$ the finite set $\{1,\ldots,n\}$ and $\mathbf{n}$ the finite based set $\{0,1,\ldots,n\}$, with zero as base-point. We write $\mathcal{N}$ for the category with objects the finite sets $\underline{n}$ for $n \geq 0$ (with $\underline{0}$ the empty set) and morphisms the maps of sets. We write $\mathcal{F}$ for the category with objects the finite based sets $\mathbf{n}$ for $n \geq 0$ and morphisms the based maps of based sets.

We typically regard a Γ-space or Γ-category as a functor from $\mathcal{F}$ to simplicial sets or categories rather than from the whole category of finite based sets.

Definition 2.2. A Γ-*space* is a functor X from $\mathcal{F}$ to simplicial sets with $X(\mathbf{0}) = *$. A map of Γ-spaces is a natural transformation of functors from $\mathcal{F}$ to simplicial sets. A Γ-*category* is a functor $\mathcal{X}$ from $\mathcal{F}$ to the category of small categories with $\mathcal{X}(\mathbf{0}) = *$, the category with the unique object $*$ and the unique morphism id_*. A map of Γ-categories is a natural transformation of functors from $\mathcal{F}$ to small categories.

We emphasize that $\mathcal{X}$ must be a strict functor to small categories: For $\phi\colon \mathbf{m} \to \mathbf{n}$ and $\psi\colon \mathbf{n} \to \mathbf{p}$, the functors $\mathcal{X}(\psi\circ\phi)$ and $\mathcal{X}(\psi)\circ\mathcal{X}(\phi)$ must be equal (and not just naturally isomorphic). A map of Γ-categories $f\colon \mathcal{X} \to \mathcal{Y}$ consists of a sequence of functors $f_n\colon \mathcal{X}(\mathbf{n}) \to \mathcal{Y}(\mathbf{n})$ such that for every map $\phi\colon \mathbf{m} \to \mathbf{n}$ in $\mathcal{F}$, the diagram

$$\begin{array}{ccc} \mathcal{X}(\mathbf{m}) & \xrightarrow{f_m} & \mathcal{Y}(\mathbf{m}) \\ {\scriptstyle \mathcal{X}(\phi)}\downarrow & & \downarrow{\scriptstyle \mathcal{Y}(\phi)} \\ \mathcal{X}(\mathbf{n}) & \xrightarrow[f_n]{} & \mathcal{Y}(\mathbf{n}) \end{array}$$

commutes strictly. In particular, applying the nerve functor objectwise to a Γ-category then produces a Γ-space. We use this in defining the "strict" homotopy theory of Γ-categories.

DEFINITION 2.3. A map $X \to Y$ of Γ-spaces is a *weak equivalence* if each map $X(\mathbf{n}) \to Y(\mathbf{n})$ is a weak equivalence of simplicial sets. A map of Γ-categories $X \to Y$ is a *weak equivalence* if the induced map $N\mathcal{X} \to N\mathcal{Y}$ is a weak equivalence of Γ-spaces.

More important than weak equivalence is the notion of stable equivalence, which for our purposes is best understood in terms of very special Γ-spaces. A Γ-space X is *special* when for each n the canonical map

$$X(\mathbf{n}) \longrightarrow X(\mathbf{1}) \times \cdots \times X(\mathbf{1}) = X(\mathbf{1})^{\times n}$$

is a weak equivalence. This canonical map is induced by the *indicator* maps $\mathbf{n} \to \mathbf{1}$ which send all but one of the non-zero element of $\mathbf{n}$ to 0. For a special Γ-space, $\pi_0 X(\mathbf{1})$ is an abelian monoid under the operation

$$\pi_0 X(\mathbf{1}) \times \pi_0 X(\mathbf{1}) \cong \pi_0 X(\mathbf{2}) \longrightarrow \pi_0 X(\mathbf{1})$$

induced by the map $\mathbf{2} \to \mathbf{1}$ sending both non-basepoint elements of $\mathbf{2}$ to the non-basepoint element of $\mathbf{1}$. A special Γ-space is *very special* when the monoid $\pi_0 X(\mathbf{1})$ is a group.

DEFINITION 2.4. A map of Γ-spaces $f\colon X \to Y$ is a *stable equivalence* when for every very special Γ-space Z, the map $f^*\colon [Y, Z] \to [X, Z]$ is a bijection, where $[-, -]$ denotes maps in the homotopy category obtained by formally inverting the weak equivalences. A map of Γ-categories $\mathcal{X} \to \mathcal{Y}$ is a *stable equivalence* when the induced map $N\mathcal{X} \to N\mathcal{Y}$ of Γ-spaces is a stable equivalence.

Equivalently, a map of Γ-spaces is a stable equivalence if and only if it induces a weak equivalence of associated spectra [4, 5.1,5.8].
In order to compare the homotopy theory of Γ-spaces and Γ-categories, we use the Fritsch-Latch-Thomason Quillen equivalence of the category of simplicial sets and the category of small categories [7, 17]. We call a map in the category of small categories a weak equivalence if it induces a weak equivalence on nerves. The nerve functor has a left adjoint "categorization functor" c, which generally does not behave well homotopically. However, $c \circ \mathrm{Sd}^2$ preserves weak equivalences, where $\mathrm{Sd}^2 = \mathrm{Sd} \circ \mathrm{Sd}$ is the second subdivision functor [8, §7].

The functor $\operatorname{Ex}^2 N$ is right adjoint to $c\operatorname{Sd}^2$, and for any simplicial set X and any category $\mathcal{C}$, the unit and counit of the adjunction,

$$X \longrightarrow \operatorname{Ex}^2 Nc\operatorname{Sd}^2 X \qquad \text{and} \qquad c\operatorname{Sd}^2\operatorname{Ex}^2 N\mathcal{C} \longrightarrow \mathcal{C},$$

are always weak equivalences. Since the natural map $X \to \operatorname{Ex}^2 X$ is always a weak equivalence and the diagrams

$$\begin{array}{ccccc} & & \operatorname{Sd}^2 X & \longrightarrow & Nc\operatorname{Sd}^2 X \\ & & \sim\downarrow & & \downarrow\sim \\ X & \xrightarrow{\sim} & \operatorname{Ex}^2\operatorname{Sd}^2 X & \longrightarrow & \operatorname{Ex}^2 Nc\operatorname{Sd}^2 X \end{array} \quad (X \xrightarrow{\sim} \operatorname{Ex}^2 Nc\operatorname{Sd}^2 X) \qquad \begin{array}{ccc} c\operatorname{Sd}^2 N\mathcal{C} & & \\ \downarrow\sim & & \\ c\operatorname{Sd}^2\operatorname{Ex}^2 N\mathcal{C} & \xrightarrow{\sim} & \mathcal{C} \end{array}$$

commute, we have natural weak equivalences

$$(2.5) \qquad Nc\operatorname{Sd}^2 X \longleftarrow \operatorname{Sd}^2 X \longrightarrow X \qquad \text{and} \qquad c\operatorname{Sd}^2 N\mathcal{C} \longrightarrow \mathcal{C}.$$

The functor Sd^2 takes the one-point simplicial set $*$ to an isomorphic simplicial set; replacing Sd^2 by an isomorphic functor if necessary, we can arrange that $\operatorname{Sd}^2 * = *$.

Definition 2.6. Let $\mathcal{S}$ be the functor from Γ-spaces to Γ-categories obtained by applying $c\operatorname{Sd}^2$ objectwise.

We then obtain the natural weak equivalences of Γ-spaces and Γ-categories (1.1) from (2.5). Inverting weak equivalences or stable equivalences, we get equivalences of homotopy categories.

Proposition 2.7. *The functors N and $\mathcal{S}$ induce inverse equivalences between the homotopy categories of Γ-spaces and Γ-categories obtained by inverting the weak equivalences.*

Proposition 2.8. *The functors N and $\mathcal{S}$ induce inverse equivalences between the homotopy categories of Γ-spaces and Γ-categories obtained by inverting the stable equivalences.*

Since both the weak equivalences and stable equivalences of Γ-spaces provide the weak equivalences in model structures (see, for example, [4]), the homotopy categories in the previous propositions are isomorphic to categories with small hom sets.

3. Review of the K-theory functor

This section reviews Segal's K-theory functor from symmetric monoidal categories to Γ-spaces and some variants of this functor. All the material in this section is well-known to experts, and most can be found in [5, 10, 11, 18]. We include it here to refer to specific details, for completeness, and to make this paper more self-contained.

For a small symmetric monoidal category $\mathcal{C}$, we typically denote the symmetric monoidal product as $\square$ and the unit as u. We construct a Γ-category $\mathcal{K}\mathcal{C}$ as follows.

Construction 3.1. Let $\mathcal{KC}(\mathbf{0}) = *$ the category with a unique object $*$ and the identity map. For $\mathbf{n}$ in $\mathcal{F}$ with $n > 0$, we define the category $\mathcal{KC}(\mathbf{n})$ to have as objects the collections $(x_I, f_{I,J})$ where

- For each subset I of $\underline{n} = \{1, \ldots, n\}$, x_I is an object of $\mathcal{C}$, and
- For each pair of disjoint subsets I, J of $\underline{n}$,

$$f_{I,J} \colon x_{I \cup J} \longrightarrow x_I \,\square\, x_J$$

is a map in $\mathcal{C}$

such that

- When I is the empty set $\emptyset$, $x_I = u$ and $f_{I,J}$ is the inverse of the unit isomorphism.
- $f_{I,J} = \gamma \circ f_{J,I}$ where γ is the symmetry isomorphism $x_J \square x_I \cong x_I \square x_J$.
- Whenever I_1, I_2, and I_3 are mutually disjoint, the diagram

$$\begin{array}{ccc} x_{I_1 \cup I_2 \cup I_3} & \xrightarrow{f_{I_1, I_2 \cup I_3}} & x_{I_1} \,\square\, x_{I_2 \cup I_3} \\ {\scriptstyle f_{I_1 \cup I_2, I_3}} \downarrow & & \downarrow {\scriptstyle \mathrm{id}\, \square f_{I_2, I_3}} \\ x_{I_1 \cup I_2} \,\square\, x_{I_3} & \xrightarrow[f_{I_1, I_2} \square \mathrm{id}]{} & x_{I_1} \,\square\, x_{I_2} \,\square\, x_{I_3} \end{array}$$

commutes (where we have omitted notation for the associativity isomorphism in $\mathcal{C}$). We write f_{I_1, I_2, I_3} for the common composite into a fixed association.

A morphism g in $\mathcal{KC}(\mathbf{n})$ from $(x_I, f_{I,J})$ to $(x'_I, f'_{I,J})$ consists of maps $h_I \colon x_I \to x'_I$ in $\mathcal{C}$ for all I such that $h_\emptyset$ is the identity and the diagram

$$\begin{array}{ccc} x_{I \cup J} & \xrightarrow{h_{I \cup J}} & x'_{I \cup J} \\ {\scriptstyle f_{I,J}} \downarrow & & \downarrow {\scriptstyle f'_{I,J}} \\ x_I \,\square\, x_J & \xrightarrow[h_I \square h_J]{} & x'_I \,\square\, x'_J \end{array}$$

commutes for all disjoint I, J.

The categories $\mathcal{KC}(\mathbf{n})$ assemble into a Γ-category as follows. For $\phi \colon \mathbf{m} \to \mathbf{n}$ in $\mathcal{F}$ and $X = (x_I, f_{I,J})$ in $\mathcal{KC}(\mathbf{m})$, define $\phi_* X = Y = (y_I, g_{I,J})$ where

$$y_I = x_{\phi^{-1}(I)} \qquad \text{and} \qquad g_{I,J} = f_{\phi^{-1}(I), \phi^{-1}(J)}$$

(replacing $*$ with u or vice-versa if $\mathbf{m}$ or $\mathbf{n}$ is $\mathbf{0}$), and likewise on maps. We obtain a Γ-space by applying the nerve functor to each category $\mathcal{KC}(\mathbf{n})$.

Definition 3.2. For a symmetric monoidal category $\mathcal{C}$, $K\mathcal{C}$ is the Γ-space $K\mathcal{C}(\mathbf{n}) = N\mathcal{KC}(\mathbf{n})$.

In terms of functoriality, $\mathcal{K}$ is obviously functorial in *strict* maps of symmetric monoidal categories, i.e., functors $F \colon \mathcal{C} \to \mathcal{D}$ that strictly preserve the product $\square$, the unit object and isomorphism, and the associativity and symmetry isomorphisms. In fact, $\mathcal{K}$ extends to a functor on the *strictly unital op-lax* maps: An *op-lax* map of symmetric monoidal categories consists of a functor $F\colon \mathcal{C} \to \mathcal{D}$, a natural transformation

$$\lambda\colon F(x \,\Box\, y) \longrightarrow F(x) \,\Box\, F(y),$$

and a natural transformation $\epsilon\colon F(u) \to u$ such that the following unit, symmetry, and associativity diagrams commute,

$$\begin{array}{ccc} F(u \,\Box\, y) & \xrightarrow{\lambda} & F(u) \,\Box\, F(y) \\ {\scriptstyle F(\eta)}\downarrow & & \downarrow{\scriptstyle \epsilon} \\ F(y) & \xleftarrow[\eta]{} & u \,\Box\, F(y) \end{array} \qquad \begin{array}{ccc} F(x \,\Box\, y) & \xrightarrow{F(\gamma)} & F(y \,\Box\, x) \\ {\scriptstyle \lambda}\downarrow & & \downarrow{\scriptstyle \lambda} \\ F(x) \,\Box\, F(y) & \xrightarrow[\gamma]{} & F(y) \,\Box\, F(x) \end{array}$$

$$\begin{array}{ccccc} & & F(x \,\Box\, y) \,\Box\, F(z) & & \\ & {\scriptstyle \lambda}\nearrow & & \searrow{\scriptstyle \lambda} & \\ F((x \,\Box\, y) \,\Box\, z) & & & & (F(x) \,\Box\, F(y)) \,\Box\, F(z) \\ {\scriptstyle F(\alpha)}\downarrow & & & & \downarrow{\scriptstyle \alpha} \\ F(x \,\Box\, (y \,\Box\, z)) & & & & F(x) \,\Box\, (F(y) \,\Box\, F(z)) \\ & {\scriptstyle \lambda}\searrow & & \nearrow{\scriptstyle \lambda} & \\ & & F(x) \,\Box\, F(y \,\Box\, z) & & \end{array}$$

where η, γ, and α denote the unit, symmetry and associativity isomorphisms, respectively. An op-lax map is *strictly unital* when the unit map ϵ is the identity (i.e., F strictly preserves the unit object). A strictly unital op-lax map $\mathcal{C} \to \mathcal{D}$ induces a map of Γ-categories $\mathcal{KC} \to \mathcal{KD}$ sending $(x_I, f_{I,J})$ in $\mathcal{KC}(\mathbf{n})$ to $(F(x_I), \lambda \circ F(f_{I,J}))$ in $\mathcal{KD}(\mathbf{n})$, and likewise for morphisms.
We will need the following additional structure in Section 5. Recall that an op-lax natural transformation $\nu\colon F \to G$ between op-lax maps is a natural transformation such that the following diagrams commute.

$$\begin{array}{ccc} F(x \,\Box\, y) & \xrightarrow{\nu} & G(x \,\Box\, y) \\ {\scriptstyle \lambda}\downarrow & & \downarrow{\scriptstyle \lambda} \\ F(x) \,\Box\, F(y) & \xrightarrow[\nu \Box \nu]{} & G(x) \,\Box\, G(y) \end{array} \qquad \begin{array}{ccc} F(u) & \xrightarrow{\nu} & G(u) \\ & {\scriptstyle \epsilon}\searrow \quad \swarrow{\scriptstyle \epsilon} & \\ & u & \end{array}$$

An op-lax natural transformation between strictly unital op-lax maps induces a natural transformation between the induced maps of Γ-categories, compatible with the Γ-structure. We summarize the discussion of the previous paragraphs in the following proposition.

Proposition 3.3. *$\mathcal{K}$ and K are functors from the category of small symmetric monoidal categories and strictly unital op-lax maps to the category of Γ-categories and the category of Γ-spaces, respectively. An op-lax natural transformation induces a natural transformation on $\mathcal{K}$ and a homotopy on K between the induced maps.*

In particular, by restricting to the subcategory consisting of the permutative categories and the strict maps, we get the functors $\mathcal{K}$ and K in the statements of the theorems in the introduction. These functors admit several variants, which extend to different variants of the category of symmetric monoidal categories.

Variant 3.4. In the construction of $\mathcal{K}$, we can require the maps $f_{I,J}$ to be isomorphisms. This is Segal's original K-theory functor as described for example in [11]. The natural domain of this functor is the category of small symmetric monoidal categories and strictly unital strong maps; these are the strictly unital op-lax maps where λ is an isomorphism.

Variant 3.5. In the construction of $\mathcal{K}$, we can require the maps $f_{I,J}$ to go the other direction, i.e.,

$$f_{I,J}\colon x_I \,\square\, x_J \longrightarrow x_{I\cup J}.$$

This is the functor called Segal K-theory in [5]; its natural domain is the category of small symmetric monoidal categories and strictly unital lax maps. A lax map $\mathcal{C} \to \mathcal{D}$ consists of a functor and natural transformations

$$\lambda\colon F(x) \,\square\, F(y) \longrightarrow F(x \,\square\, y) \qquad \text{and} \qquad \epsilon\colon u \longrightarrow F(u)$$

making the evident unit, symmetry, and associativity diagrams commute. Put another way, (F, λ, ϵ) defines an op-lax map $\mathcal{C} \to \mathcal{D}$ if and only if $(F^{\mathrm{op}}, \lambda, \epsilon)$ defines a lax map $\mathcal{C}^{\mathrm{op}} \to \mathcal{D}^{\mathrm{op}}$.

We also have variants which loosen the unit condition, but the constructions occur most naturally by way of functors between different categories of small symmetric monoidal categories. The inclusion of the category with strictly unital op-lax maps into the category with op-lax maps has a left adjoint U. Concretely, $U\mathcal{C}$ has objects the objects of $\mathcal{C}$ plus a new disjoint object v. Morphisms in $U\mathcal{C}$ between objects of $\mathcal{C}$ are just the morphisms in $\mathcal{C}$, and morphisms to and from v are defined by

$$U\mathcal{C}(x, v) = \mathcal{C}(x, u), \qquad U\mathcal{C}(v, x) = \emptyset, \qquad U\mathcal{C}(v, v) = \{\mathrm{id}_v\},$$

for x an object of $\mathcal{C}$ and u the unit in $\mathcal{C}$. We obtain a symmetric monoidal product on $U\mathcal{C}$ from the symmetric monoidal product on $\mathcal{C}$ with v chosen to be a strict unit (i.e., $v \,\square\, x = x$ for all x in $U\mathcal{C}$); the inclusion of $\mathcal{C}$ in $U\mathcal{C}$ is then op-lax monoidal and the functor $U\mathcal{C} \to \mathcal{C}$ sending v to u is strictly unital op-lax (in fact, strict). Then $\mathcal{K} \circ U$ defines a functor from the category of small symmetric monoidal categories and op-lax maps to Γ-categories.

To compare these variants and to understand K, we construct weak equivalences

$$p_n\colon \mathcal{K}\mathcal{C}(\mathbf{n}) \longrightarrow \mathcal{C} \times \cdots \times \mathcal{C} = \mathcal{C}^{\times n}. \tag{3.6}$$

Define p_n to be the functor sends the object $(x_I, f_{I,J})$ of $\mathcal{KC}(n)$ to the object $(x_{\{1\}}, \dots, x_{\{n\}})$ of $\mathcal{C}^{\times n}$, and likewise for maps. This functor has a right adjoint q_n that sends $(y_1, \dots, y_n)$ to the system $(x_I, f_{I,J})$ with

$$x_{\{i_1,\dots,i_r\}} = (\cdots(y_{i_1} \Box y_{i_2}) \Box \cdots) \Box y_{i_r}$$

for $i_1 < \cdots < i_r$ and the maps $f_{I,J}$ induced by the associativity and symmetry isomorphisms. In the case $n = 1$, these are inverse isomorphisms of categories, and under these isomorphisms, (3.6) is induced by the indicator maps $\mathbf{n} \to \mathbf{1}$. Because an adjunction induces inverse homotopy equivalences on nerves, this proves the following proposition.

Proposition 3.7. *For any small symmetric monoidal category $\mathcal{C}$, $K\mathcal{C}$ is a special Γ-space with $K\mathcal{C}(\mathbf{1})$ isomorphic to $N\mathcal{C}$.*

Similar observations apply to the variant functors above. We have natural transformations relating the strictly unital strong construction to both the strictly unital lax and op-lax constructions. It follows that the K-theory Γ-spaces obtained are naturally weakly equivalent. Likewise, the constructions with the weakened units map to the constructions with strict units. Since the map $U\mathcal{C} \to \mathcal{C}$ induces a homotopy equivalence on nerves, these natural transformations induce natural weak equivalences of Γ-spaces.

Recall that we say that a functor between small categories is a *weak equivalence* when it induces a weak equivalence on nerves. As a consequence of the previous proposition, the K-theory functor preserves weak equivalences. As in the introduction, we say that a strictly unital op-lax map of symmetric monoidal categories is a *stable equivalence* if it induces a stable equivalence on K-theory Γ-spaces, or equivalently, if it induces a weak equivalence on the group completion of the nerves. Quillen's homological criterion to identify the group completion [13] then applies to give an intrinsic characterization of the stable equivalences.

Proposition 3.8. *A map of symmetric monoidal categories $\mathcal{C} \to \mathcal{D}$ is a stable equivalence if and only if it induces an isomorphism of localized homology rings*

$$H_*\mathcal{C}[(\pi_0\mathcal{C})^{-1}] \longrightarrow H_*\mathcal{D}[(\pi_0\mathcal{D})^{-1}]$$

obtained by inverting the multiplicative monoids $\pi_0\mathcal{C} \subset H_0\mathcal{C}$ and $\pi_0\mathcal{D} \subset H_0\mathcal{D}$.

Although not needed in what follows, for completeness of exposition, we offer the following well-known observation on the homotopy theory of the various categories of symmetric monoidal categories. Recall that we say that a functor between small categories is a *weak equivalence* when it induces a weak equivalence on nerves. The following theorem can be proved using the methods of [10, 4.2] and [6, 4.2].

Theorem 3.9. *The following homotopy categories are equivalent:*

(i) *The homotopy category obtained from the category of small permutative categories and strict maps by inverting the weak equivalences.*

(ii) *The homotopy category obtained from the category of small symmetric monoidal categories and strict maps by inverting the weak equivalences.*
(iii) *The homotopy category obtained from the category of small symmetric monoidal categories and strictly unital strong maps by inverting the weak equivalences.*
(iv) *The homotopy category obtained from the category of small symmetric monoidal categories and strictly unital op-lax maps by inverting the weak equivalences.*
(v) *The homotopy category obtained from the category of small symmetric monoidal categories and strictly unital lax maps by inverting the weak equivalences.*

4. Construction of the inverse K-theory functor

In this section we construct the inverse K-theory functor $\mathcal{P}$ as a Grothendieck construction (or homotopy colimit) over a category $\mathcal{A}$ described below. We construct the natural transformations displayed in (1.2) relating the composites $\mathcal{KP}$ and $\mathcal{PK}$ with the identity. This section contains only the constructions; we postpone almost all homotopical analysis to the next section.
We begin with the construction of the category $\mathcal{A}$. As indicated in the introduction, we define the objects of $\mathcal{A}$ to consist of the sequences of positive integers $(n_1,\dots,n_s)$ for all $s\geq 0$, with $s=0$ corresponding to the empty sequence $()$. We think of each n_i as the finite (unbased) set $\underline{n}_i$, and we define the maps in $\mathcal{A}$ to be the maps generated by maps of finite sets, permutations in the sequence, and partitioning $\underline{n}_i$ into subsets. We make this precise in the following definition.

Definition 4.1. For $\vec{m}=(m_1,\dots,m_r)$ and $\vec{n}=(n_1,\dots,n_s)$ with $r,s>0$, we define the morphisms $\mathcal{A}(\vec{m},\vec{n})$ to be the subset of the maps of finite (unbased) sets

$$\underline{m}_1\amalg\cdots\amalg\underline{m}_r\longrightarrow\underline{n}_1\amalg\cdots\amalg\underline{n}_s$$

satisfying the property that the inverse image of each subset $\underline{n}_j$ is either empty or contained in a single $\underline{m}_i$ (depending on j). For the object $()$, we define $\mathcal{A}((),\vec{n})$ consist of a single point for all $\vec{n}$ in $\mathcal{A}$ and we define $\mathcal{A}(\vec{m},())$ to be empty for $\vec{m}\neq()$.

For a Γ-category $\mathcal{X}$, let $A\mathcal{X}()=\mathcal{X}(\mathbf{0})$ and

$$A\mathcal{X}(n_1,\dots,n_s)=\mathcal{X}(\mathbf{n}_1)\times\cdots\times\mathcal{X}(\mathbf{n}_s).$$

For a map $\phi\colon\vec{m}\to\vec{n}$ in $\mathcal{A}$, define

$$A\phi\colon\mathcal{X}(\mathbf{m}_1)\times\cdots\times\mathcal{X}(\mathbf{m}_r)\longrightarrow\mathcal{X}(\mathbf{n}_1)\times\cdots\times\mathcal{X}(\mathbf{n}_s)$$

as follows. If $s=0$, then $r=0$ and ϕ is the identity, and we take $A\phi$ to be the identity. If $r=0$ and $s>0$, we take $A\phi$ to be the map $\mathcal{X}(\mathbf{0})\to\mathcal{X}(\mathbf{n}_j)$ on each coordinate. If $r>0$, then by definition, for each j, the subset $\underline{n}_j$ of

$$\underline{n}_1\amalg\cdots\amalg\underline{n}_s$$

has inverse image either empty or contained in a single $\underline{m}_i$ for some i; if the inverse image is non-empty, then ϕ restricts to a map of unbased sets $\underline{m}_i \to \underline{n}_j$, which we extend to a map of based sets $\mathbf{m}_i \to \mathbf{n}_j$ that is the identity on the basepoint 0. In this case, we define $A\phi$ on the j-th coordinate to be the composite of the projection

$$\mathcal{X}(\mathbf{m}_1) \times \cdots \times \mathcal{X}(\mathbf{m}_r) \longrightarrow \mathcal{X}(\mathbf{m}_i)$$

and the map $\mathcal{X}(\mathbf{m}_i) \to \mathcal{X}(\mathbf{n}_j)$ induced by the restriction of ϕ. In the case when the inverse image of $\underline{n}_j$ is empty, we define $A\phi$ on the j-th coordinate to be the composite of the projection

$$\mathcal{X}(\mathbf{m}_1) \times \cdots \times \mathcal{X}(\mathbf{m}_r) \longrightarrow * = \mathcal{X}(\mathbf{0})$$

and the map $\mathcal{X}(\mathbf{0}) \to \mathcal{X}(\mathbf{n}_j)$. An easy check gives the following observation.

PROPOSITION 4.2. *A is a functor from the category of small Γ-categories to the category of functors from $\mathcal{A}$ to the category of small categories.*

We can now define the functors $\mathcal{P}$ and P, at least on the level of functors to small categories.

DEFINITION 4.3. Let $\mathcal{P}\mathcal{X} = \mathcal{A} \int A\mathcal{X}$. Let $P = \mathcal{P} \circ \mathcal{S}$.

More concretely, the category $\mathcal{P}\mathcal{X}$ has as objects the disjoint union of the objects of $A\mathcal{X}(\vec{n})$ where $\vec{n}$ varies over the objects of $\mathcal{A}$. For $x \in A\mathcal{X}(\vec{m})$ and $y \in A\mathcal{X}(\vec{n})$, a map in $\mathcal{P}\mathcal{X}$ from x to y consists of a map $\phi\colon \vec{m} \to \vec{n}$ in $\mathcal{A}$ together with a map $\phi_* x \to y$ in $A\mathcal{X}(\vec{n})$, where $\phi_* = A\phi$ is the functor $A\mathcal{X}(\vec{m}) \to A\mathcal{X}(\vec{n})$ above.

Variant 4.4. We can regard $A\mathcal{X}$ as a contravariant functor on $\mathcal{A}^{\mathrm{op}}$ and form the contravariant Grothendieck construction $\mathcal{P}^{\mathrm{lax}}\mathcal{X} = \mathcal{A}^{\mathrm{op}} \int A\mathcal{X}$. This has the same objects as $\mathcal{P}\mathcal{X}$ but for $x \in A\mathcal{X}(\vec{m})$ and $y \in A\mathcal{X}(\vec{n})$, a map in $\mathcal{P}^{\mathrm{lax}}\mathcal{X}$ from x to y consists of a map $\phi\colon \vec{n} \to \vec{m}$ in $\mathcal{A}$ together with a map $x \to \phi_* y$. This functor is better adapted to the category of symmetric monoidal categories and strictly unital lax maps. All results and constructions in this paper admit analogues for $\mathcal{P}^{\mathrm{lax}}$, replacing "op-lax" with "lax" in the work below.

The category $\mathcal{A}$ has the structure of a permutative category under concatenation of sequences, with the empty sequence as the unit and the symmetry morphisms induced by permuting elements in the sequences. The category of small categories is symmetric monoidal under cartesian product and the functor $A\mathcal{X}\colon \mathcal{A} \to \mathbf{Cat}$ associated to a Γ-category $\mathcal{X}$ is a strong symmetric monoidal functor. For formal reasons, then the Grothendieck construction $\mathcal{P}\mathcal{X}$ naturally obtains the structure of a symmetric monoidal category; we can describe this structure concretely as follows. For any object x in $A\mathcal{X}(\vec{m})$, we can write $x = (x_1, \ldots, x_r)$ for objects x_i in $\mathcal{X}(\mathbf{m}_i)$; then for y in $A\mathcal{X}(\vec{n})$,

$$x \,\square\, y = (x_1, \ldots, x_r, y_1, \ldots, y_s) \in \mathrm{Ob}\, A\mathcal{X}(m_1, \ldots, m_r, n_1, \ldots, n_s),$$

where we understand the unique object of $A\mathcal{X}()$ as a strict unit. The product on maps admits an analogous description. This concrete description makes it clear that $\mathcal{PX}$ is in fact a permutative category. Moreover, a map $\mathcal{X} \to \mathcal{Y}$ of Γ-categories induces a strict map of permutative categories $\mathcal{PX} \to \mathcal{PY}$. We obtain the following theorem.

Theorem 4.5. *$\mathcal{P}$ defines a functor from the category of Γ-categories to the category of permutative categories and strict maps.*

Next we construct the natural transformations of (1.2). Starting with a symmetric monoidal category $\mathcal{C}$, we construct the map $\mathcal{PKC} \to \mathcal{C}$ using the homotopy colimit property of the Grothendieck construction. Specifically, we construct functors $\alpha_{\vec{m}}$ from $A\mathcal{PKC}(\vec{m})$ to $\mathcal{C}$ and suitably compatible natural transformations for the maps in $\mathcal{A}$.

For each $\vec{m}$ in $\mathcal{A}$, define the functor

$$\alpha_{\vec{m}} \colon A\mathcal{KC}(\vec{m}) = \mathcal{KC}(\mathbf{m}_1) \times \cdots \times \mathcal{KC}(\mathbf{m}_r) \longrightarrow \mathcal{C}$$

to take the object $\vec{X} = (X_1, \ldots, X_r)$ to

$$(\cdots (x^1_{\underline{m}_1} \,\Box\, x^2_{\underline{m}_2}) \,\Box\, \cdots) \,\Box\, x^r_{\underline{m}_r}$$

where $X_i = (x^i_I, f_{I,J})$ for $I \subset \underline{m}_i$, and likewise for maps in $\mathcal{KC}(\vec{m})$. For $\vec{m} = ()$, we understand $\alpha_{()}$ to include the category $A\mathcal{KC}() = *$ in $\mathcal{C}$ as the unit u and the identity on u.

For a map ϕ in $\mathcal{A}$ from $\vec{m}$ to $\vec{n}$, define

$$\alpha_\phi \colon \alpha_{\vec{m}}(y_1, \ldots, y_r) \longrightarrow \alpha_{\vec{n}}(\phi_*(y_1, \ldots, y_r))$$

to be the map induced by the associativity, symmetry, and inverse unit isomorphisms in $\mathcal{C}$ and the maps $f^i_{I_1,\ldots,I_k}$ in y_i: if ϕ sends $\underline{m}_i$ into $\underline{n}_{j_1}, \ldots, \underline{n}_{j_t}$, then composing maps $f^i_{I,J}$ in y_i gives a well-defined map

$$f_{I_1,\ldots,I_t} \colon x^i_{\underline{m}_i} \longrightarrow (\cdots (x^i_{I_1} \,\Box\, x^i_{I_2}) \,\Box\, \cdots) \,\Box\, x^i_{I_t}$$

where I_k is the subset of $\underline{m}_i$ landing in $\underline{n}_{j_k}$. The map α_ϕ is a natural transformation of functors from $\alpha_{\vec{m}}$ to $\alpha_{\vec{n}} \circ \phi_*$. Moreover, given a map ψ from $\vec{n}$ to $\vec{p}$ in $\mathcal{A}$, the following diagram commutes

$$\begin{array}{ccc}
\alpha_{\vec{m}}\vec{X} & \xrightarrow{\alpha_\phi} & \alpha_{\vec{n}}(\phi_*\vec{X}) \\
{\scriptstyle \alpha_{\psi\circ\phi}}\downarrow & & \downarrow{\scriptstyle \alpha_\psi} \\
\alpha_{\vec{p}}((\psi \circ \phi)_*\vec{X}) & = & \alpha_{\vec{p}}(\psi_*\phi_*\vec{X})
\end{array}$$

for any $\vec{X}$ in $A\mathcal{PKC}(\vec{m})$.

Definition 4.6. Let $\alpha \colon \mathcal{PKC} \to \mathcal{C}$ be the functor $\mathcal{A} \int AX \to \mathcal{KC}$ that sends $\vec{X}$ in $A\mathcal{KC}(\vec{m})$ to $\alpha_{\vec{m}}\vec{X}$ and sends the map

$$\phi \colon \vec{m} \longrightarrow \vec{n}, \quad f \colon \phi_*\vec{X} \longrightarrow \vec{Y}$$

to the map $\alpha_{\vec{n}}(f) \circ \alpha_\phi$ in $\mathcal{C}$.

Examining the construction of α and the symmetric monoidal structure on $\mathcal{PKC}$, we obtain the following theorem.

Theorem 4.7. *The functor* $\alpha\colon \mathcal{PKC} \to \mathcal{C}$ *satisfies the following properties.*

(i) α *is a strictly unital strong map of symmetric monoidal categories.*
(ii) α *is natural up to natural transformation in strictly unital op-lax maps.*
(iii) α *is a strict map when* $\mathcal{C}$ *is a permutative category.*
(iv) α *is natural in strict maps.*

The meaning of (ii) and (iv) is that for a strictly unital op-lax map $F\colon \mathcal{C} \to \mathcal{D}$, the diagram

$$\begin{array}{ccc} \mathcal{PKC} & \longrightarrow & \mathcal{PKD} \\ \downarrow{\scriptstyle\alpha} & & \downarrow{\scriptstyle\alpha} \\ \mathcal{C} & \longrightarrow & \mathcal{D} \end{array}$$

commutes up to natural transformation, namely, the natural transformation

$$\lambda\colon F(x_1 \,\square \cdots \square\, x_r) \longrightarrow F(x_1) \,\square \cdots \square\, F(x_r)$$

which is part of the structure of the op-lax map. When $\mathcal{C} \to \mathcal{D}$ is a strict map, the diagram commutes strictly (the natural transformation is the identity).

For the remaining natural transformation in (1.2), note that for a Γ-category $\mathcal{X}$, we have a canonical inclusion $\iota\colon \mathcal{X}(\mathbf{n}) \to \mathcal{KPX}(\mathbf{n})$ sending an object x in $\mathcal{X}(\mathbf{n})$ to the object $\iota x = (x_I, f_{I,J})$ in $\mathcal{KPX}(\mathbf{n})$ with

$$x_I = \pi^I_*(x) \in \mathcal{X}(\mathbf{m}) = A\mathcal{X}(m)$$

for $m = |I|$, $I = \{i_1, \ldots, i_m\}$ with $i_1 < \cdots < i_m$, and $\pi^I\colon \mathbf{n} \to \mathbf{m}$ the map that sends i_k to k and every other element of $\mathbf{n}$ to 0. The map

$$f_{I,J}\colon x_{I\cup J} \longrightarrow x_I \,\square\, x_J = (x_I, x_J) \in A\mathcal{X}(|I|, |J|)$$

is induced by the map $(|I \cup J|) \to (|I|, |J|)$ in $\mathcal{A}$ corresponding to the partition of the ordered set $I \cup J$ into I and J. This does not fit together into a map of Γ-categories: For a map $\phi\colon \mathbf{m} \to \mathbf{n}$ in $\mathcal{F}$,

$$\iota(\phi_* x)_I = \pi^I_*(\phi_* x), \qquad \text{but} \qquad \phi_*(\iota x)_I = \pi^{\phi^{-1}I}_*(x).$$

Writing ϕ' for the map in $\mathcal{N}$ corresponding to the restriction of ϕ to the map $\phi^{-1}I \to I$, then

$$\pi^I \circ \phi = \phi' \circ \pi^{\phi^{-1}I}$$

in $\mathcal{F}$. We can interpret ϕ' as a map

$$\pi^{\phi^{-1}I}_*(x) \longrightarrow \pi^I_*(\phi_* x)$$

in $\mathcal{PX}$. These maps in turn assemble to a map

$$\omega_\phi\colon \phi_*\iota x \longrightarrow \iota\phi_* x$$

in $\mathcal{KPX}$, natural in x.

Definition 4.8. For a Γ-category $\mathcal{X}$, let $\mathcal{WX}(\mathbf{n})$ be the category whose objects consist of triples (y, x, g) with y an object of $\mathcal{KP}(\mathbf{n})$, x an object of $\mathcal{X}(\mathbf{n})$ and

$g\colon y \to \iota x$ a map in $\mathcal{KP}(\mathbf{n})$. The morphisms of $\mathcal{WX}(\mathbf{n})$ are the commuting diagrams. For $\phi\colon \mathbf{m} \to \mathbf{n}$ in $\mathcal{F}$, define

$$\mathcal{WX}(\phi)\colon \mathcal{WX}(\mathbf{m}) \longrightarrow \mathcal{WX}(\mathbf{n})$$

to be the functor that takes (y, x, g) to $(\phi_* y, \phi_* x, \omega_\phi \circ \phi_* g)$.

We note for later use that for (y, x, g) an object in $\mathcal{WX}(\mathbf{n})$, writing $y = (y_I, f_{I,J})$ with y_I in $\mathcal{PX}$, we must have each y_I in $A\mathcal{X}()$ or $A\mathcal{X}(m_I)$ for some m_I. This is because ιx_I is in $A\mathcal{X}(n)$ and maps in $\mathcal{A}$ cannot decrease the length of the sequence.

We claim that the categories $\mathcal{WX}(\mathbf{n})$ and functors $\mathcal{WX}(\phi)$ assemble into a Γ-category. For $\phi\colon \mathbf{m} \to \mathbf{n}$, $\psi\colon \mathbf{n} \to \mathbf{p}$, and $I \subset \underline{p}$, write

$$\pi^I \circ \psi \circ \phi = \psi' \circ \pi^{\psi^{-1}I} \circ \phi = \psi' \circ \phi' \circ \pi^{\phi^{-1}(\psi^{-1}I)}$$

as above, with $\psi'\colon \psi^{-1}I \to I$ and $\phi'\colon \phi^{-1}(\psi^{-1}I) \to \psi^{-1}I$ the restrictions of ψ and ϕ, using the natural order on $I \subset \underline{p}$, $\psi^{-1}I \subset \underline{n}$, and $\phi^{-1}(\psi^{-1}I) \subset \underline{m}$ to view these as maps in $\mathcal{F}$. Then $\psi' \circ \phi'\colon (\psi \circ \phi)^{-1}I \to I$ is the restriction of $\psi \circ \phi$; this is the check required to see that the diagram

$$\begin{array}{ccc} \pi_*^{(\psi\circ\phi)^{-1}I} x & \longrightarrow & \pi_*^{\psi^{-1}I}(\phi_* x) \\ & \searrow \quad \swarrow & \\ & \pi_*^I((\psi \circ \phi)_* x) & \end{array}$$

in $\mathcal{PX}$ commutes. Examination of the structure maps $f_{I,J}$ in ιx shows that the diagram

$$\begin{array}{ccc} (\psi \circ \phi)_* \iota x & \xrightarrow{\psi_* \omega_\phi} & \psi_* \iota(\phi_* x) \\ & {\scriptstyle \omega_{\psi\circ\phi}} \searrow \quad \swarrow {\scriptstyle \omega_\psi} & \\ & \iota((\psi \circ \phi)_* x) & \end{array}$$

in $\mathcal{KPX}$ commutes. This proves the following theorem.

Theorem 4.9. *The maps $\mathcal{WX}(\phi)$ above make $\mathcal{WX}$ into a Γ-category.*

Since $\mathcal{WX}$ is natural in maps of Γ-categories $\mathcal{X}$, we can regard $\mathcal{W}$ as an endofunctor on Γ-categories. By construction, the forgetful functors $\omega\colon \mathcal{WX} \to \mathcal{X}$ and $\upsilon\colon \mathcal{WX} \to \mathcal{KPX}$ are natural transformations of endofunctors. For fixed $\mathbf{n}$, the functor $\mathcal{WX}(\mathbf{n}) \to \mathcal{X}(\mathbf{n})$ is a left adjoint: The right adjoint sends x in $\mathcal{X}(\mathbf{n})$ to $(\iota x, x, \mathrm{id}_{\iota x})$ in $\mathcal{WX}(\mathbf{n})$. It follows that ω is always a weak equivalence of Γ-categories. We summarize this in the following theorem.

Theorem 4.10. *The maps $\upsilon\colon \mathcal{WX} \to \mathcal{KPX}$ and $\omega\colon \mathcal{WX} \to \mathcal{X}$ are natural transformations of endofunctors on Γ-categories, and ω is a weak equivalence for any $\mathcal{X}$.*

5. Proof of Theorems 1.3 and 1.4

This section provides the homotopical analysis of the functors and natural transformations constructed in the previous section. This leads directly to the proof of the main theorem, Theorem 1.3, and its non-completed variant, Theorem 1.4.

Most of the arguments hinge on the following lemma of Thomason [16]:

Lemma 5.1 (Thomason). *Let $\mathcal{A}$ be a small category and F a functor from $\mathcal{A}$ to the category of small categories. There is a natural weak equivalence of simplicial sets*

$$\operatorname{hocolim}_{\mathcal{A}} NF \longrightarrow N(\mathcal{A} \textstyle\int F).$$

The natural transformation is easy to describe. We write an object of $\mathcal{A} \int F$ as $(\vec{n}, x)$ with $\vec{n}$ an object of $\mathcal{A}$ and x an object of $F\vec{n}$, and we write a map in $\mathcal{A} \int F$ as $(\phi, f)\colon (\vec{n}, x) \to (\vec{p}, y)$ where $\phi\colon \vec{n} \to \vec{p}$ is a map in $\mathcal{A}$ and $f\colon F(\phi)(x) \to y$ is a map in $F\vec{p}$. Then a q-simplex of the nerve $N(\mathcal{A} \int F)$ is a sequence of q composable maps

$$(\vec{n}_0, x_0) \xrightarrow{(\phi_1, f_1)} (\vec{n}_1, x_1) \xrightarrow{(\phi_2, f_2)} \cdots \xrightarrow{(\phi_q, f_q)} (\vec{n}_q, x_q).$$

Likewise, a q-simplex in the homotopy colimit consists of a sequence of q composable maps in $\mathcal{A}$ together with q composable maps in $F(\vec{n}_0)$:

$$\vec{n}_0 \xrightarrow{\phi_1} \vec{n}_1 \xrightarrow{\phi_2} \cdots \xrightarrow{\phi_q} \vec{n}_q$$

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} \cdots \xrightarrow{f_q} x_q.$$

The natural transformation sends this simplex of the homotopy colimit to the simplex

$$(\vec{n}_0, x_0) \xrightarrow{(\phi_1, f_1)} (\vec{n}_1, x_1') \xrightarrow{(\phi_2, f_2')} \cdots \xrightarrow{(\phi_q, f_q')} (\vec{n}_q, x_q'),$$

where $x_k' = F(\phi_{k,\ldots,1})(x_k)$ and $f_k' = F(\phi_{k-1,\ldots,1})(f_k)$ for $\phi_{k,\ldots,1} = \phi_k \circ \cdots \circ \phi_1$. A Quillen Theorem A style argument proves that this map is a weak equivalence [16, §1.2].

Applying Thomason's lemma to the Grothendieck construction $\mathcal{A} \int A\mathcal{X}$, we get the following immediate observation.

Proposition 5.2. *$\mathcal{P}$ preserves weak equivalences.*

The following theorem provides the main homotopical result we need for the remaining arguments in this section.

Theorem 5.3. *Let $\mathcal{X}$ be a special Γ-category. Then the inclusion of $\mathcal{X}(\mathbf{1})$ in $\mathcal{P}\mathcal{X}$ is a weak equivalence.*

Proof. Recall that $\mathcal{N}$ denotes the category with objects $\underline{n} = \{1, \ldots, n\}$ and morphisms the maps of sets. We have an inclusion $\eta\colon \mathcal{N} \to \mathcal{A}$ sending $\underline{0}$ to $()$ and $\underline{n}$ to (n) for $n > 0$. We have a functor $\epsilon\colon \mathcal{A} \to \mathcal{N}$ sending $\vec{n} = (n_1, \ldots, n_s)$

to $\underline{n}$ with $n = n_1 + \cdots + n_s$. Let $B\mathcal{X}$ be the functor from $\mathcal{A}$ to small categories defined by

$$B\mathcal{X}(\vec{n}) = \epsilon^*\mathcal{X}(\vec{n}) = \mathcal{X}(\epsilon(\vec{n})) = \mathcal{X}(\mathbf{n}).$$

Then the maps $\mathbf{n} \to \mathbf{n}_j$ coming from the partition of n as $\vec{n}$ induce a natural transformation of functors $B\mathcal{X} \to A\mathcal{X}$. The hypothesis that $\mathcal{X}$ is special implies that this map is an objectwise weak equivalence. Now applying Thomason's lemma, it suffices to show that the inclusion of $N\mathcal{X}(\mathbf{1})$ in $\operatorname{hocolim}_{\mathcal{A}} NB\mathcal{X}$ is a weak equivalence.

Since $B\mathcal{X} = \epsilon^*\mathcal{X}$ as a functor on $\mathcal{A}$ and $\mathcal{X} = \eta^* B\mathcal{X}$ as a functor on $\mathcal{N}$, we have canonical maps

$$\operatorname{hocolim}_{\mathcal{N}} N\mathcal{X} \longrightarrow \operatorname{hocolim}_{\mathcal{A}} NB\mathcal{X} \longrightarrow \operatorname{hocolim}_{\mathcal{N}} N\mathcal{X} \tag{5.4}$$

induced by ϵ and η. The composite map on $\operatorname{hocolim}_{\mathcal{N}} N\mathcal{X}$ is induced by $\epsilon \circ \eta = \mathrm{Id}_{\mathcal{N}}$, and is therefore the identity. The composite map on $\operatorname{hocolim}_{\mathcal{A}} NB\mathcal{X}$ is induced by $\eta \circ \epsilon$. We have a natural transformation from $\eta \circ \epsilon$ to the identity functor on $\mathcal{A}$ induced by the partition maps,

$$\eta \circ \epsilon(\vec{n}) = (n) \longrightarrow (n_1, \ldots, n_s) = \vec{n}.$$

Because

$$B\mathcal{X}(\eta \circ \epsilon(\vec{n})) = \mathcal{X}(\mathbf{n}) = B\mathcal{X}(\vec{n}),$$

we get a homotopy from the composite map on $\operatorname{hocolim}_{\mathcal{A}} NB\mathcal{X}$ to the identity. In other words, we have shown that the maps in (5.4) are inverse homotopy equivalences. Since $\underline{1}$ is the final object in $\mathcal{N}$, the inclusion of $N\mathcal{X}(\mathbf{1})$ in $\operatorname{hocolim}_{\mathcal{N}} N\mathcal{X}$ is a homotopy equivalence, and it follows that the inclusion of $N\mathcal{X}(\mathbf{1})$ in $\operatorname{hocolim}_{\mathcal{A}} NB\mathcal{X}$ is a homotopy equivalence. □

When $\mathcal{X} = \mathcal{KC}$ for a small symmetric monoidal category $\mathcal{C}$, we have the canonical isomorphism $\mathcal{KC}(\mathbf{1}) \cong \mathcal{C}$, and the composite map

$$\mathcal{C} \cong \mathcal{KC}(\mathbf{1}) \longrightarrow \mathcal{PKC} \longrightarrow \mathcal{C}$$

is the identity on $\mathcal{C}$. Since $\mathcal{KC}$ is always a special Γ-category, we get the following corollary.

Corollary 5.5. *The natural map $\alpha\colon \mathcal{PKC} \to \mathcal{C}$ is always a weak equivalence.*

We also get a comparison for $\mathcal{KPX}$ when $\mathcal{X}$ is special.

Corollary 5.6. *If $\mathcal{X}$ is special, then $\upsilon\colon \mathcal{WX} \to \mathcal{KPX}$ is a weak equivalence.*

Proof. Let $\mathcal{X}$ be a special Γ-category. The restriction of the map ω to the $\mathbf{1}$-categories, $\mathcal{WX}(\mathbf{1}) \to \mathcal{X}(\mathbf{1})$, is an equivalence of categories, and the composite map

$$\mathcal{X}(\mathbf{1}) \longrightarrow \mathcal{WX}(\mathbf{1}) \longrightarrow \mathcal{KPX}(\mathbf{1}) = \mathcal{PX}$$

is the map in the theorem, and therefore a weak equivalence. It follows that the restriction of υ to the $\mathbf{1}$-categories is a weak equivalence. Since the map $\omega\colon \mathcal{WX} \to \mathcal{X}$ is a weak equivalence, $\mathcal{WX}$ is also a special Γ-category, and it follows that υ is a weak equivalence. □

Together with Proposition 2.7 and Theorem 4.10, Corollaries 5.5 and 5.6 prove Theorem 1.4. To prove Theorem 1.3, we need to see that the map υ is always a stable equivalence. For this we use the following technical lemma.

Lemma 5.7. *The diagram*

$$\begin{array}{ccccc} \mathcal{WKPX} & \xrightarrow{\upsilon} & \mathcal{KPKPX} & \xleftarrow{\mathcal{KP}\upsilon} & \mathcal{KPWX} \\ & {\scriptstyle\omega}\searrow & \downarrow{\scriptstyle\mathcal{K}\alpha} & \swarrow{\scriptstyle\mathcal{KP}\omega} & \\ & & \mathcal{KPX} & & \end{array}$$

commutes up to natural transformation of maps of Γ*-categories. All maps in the diagram are weak equivalences.*

Proof. The weak equivalence statement follows from the diagram statement since α and ω are always weak equivalences and $\mathcal{K}$ and $\mathcal{P}$ preserve weak equivalences. For the diagram statement, it suffices to show that the diagrams

$$\begin{array}{ccc} \mathcal{WKC} & \xrightarrow{\upsilon} & \mathcal{KPKC} \\ & {\scriptstyle\omega}\searrow & \downarrow{\scriptstyle\mathcal{K}\alpha} \\ & & \mathcal{KC} \end{array} \qquad \begin{array}{ccc} \mathcal{PKPX} & \xleftarrow{\mathcal{P}\upsilon} & \mathcal{PWX} \\ {\scriptstyle\alpha}\downarrow & \swarrow{\scriptstyle\mathcal{P}\omega} & \\ \mathcal{PX} & & \end{array}$$

commute up to natural transformation of maps of Γ-categories (on the left) for all $\mathcal{C}$ and up to op-lax natural transformation (on the right) for all $\mathcal{X}$.

On the left, starting with an object (y, x, g) in $\mathcal{WKC}(\mathbf{n})$, the top left composite takes this to $\mathcal{K}\alpha(y)$ and the diagonal arrow takes this to x; the effect on maps in $\mathcal{WKC}(\mathbf{n})$ admits the analogous description. Since $\mathcal{K}\alpha(\iota x) = x$, $\mathcal{K}\alpha(g)$ is a map from $\mathcal{K}\alpha(y)$ to x, which is natural in $\mathcal{WKC}(\mathbf{n})$, and compatible with the Γ-structure.

On the right, consider an element $X = (X_1, \ldots, X_s)$ in $A\mathcal{WX}(\vec{n})$, where $X_i = (y^i, x^i, g^i)$ is an object in $\mathcal{WX}(\mathbf{n}_i)$. As per the remark following Definition 4.8, we can write $y^i = (y^i_I, f_{I,J})$ for y^i_I some object of $\mathcal{X}(\mathbf{m}_I)$ (thought of as $A\mathcal{X}(m)$ or $A\mathcal{X}()$) for some m_I, where I ranges over the subsets of $\underline{n}_i$. The left down composite sends X to

$$\alpha(y^1, \ldots, y^s) = (y^1_{\underline{m}_{\underline{n}_1}}, \ldots, y^s_{\underline{m}_{\underline{n}_s}})$$

since the symmetric monoidal product in $\mathcal{PX}$ is concatenation. An analogous description applies to maps of X in $\mathcal{PWX}$. The diagonal in the diagram sends X to $(x^1, \ldots, x^s)$ and we have the map

$$(g^i_{\underline{m}_{\underline{n}_i}})\colon (y^i_{\underline{m}_{\underline{n}_i}}) \longrightarrow (\iota x^i_{\underline{m}_{\underline{n}_i}}) = (x^i).$$

in $\mathcal{PX}$. This map is natural in X in $\mathcal{PWX}$ and is a strictly monoidal natural transformation. □

Proof of Theorem 1.3. Given Propositions 2.7 and 2.8, Theorem 4.10, and Corollaries 5.5 and 5.6, it suffices to show that the map $\upsilon\colon \mathcal{WX} \to \mathcal{KPX}$

is always a stable equivalence. Writing $[-,-]$ for maps in the homotopy category obtained by formally inverting the weak equivalences, we need to show that

$$v^*\colon [\mathcal{KPX},\mathcal{Z}] \longrightarrow [\mathcal{WX},\mathcal{Z}]$$

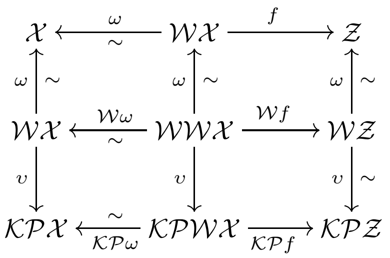
is a bijection for every very special Γ-category $\mathcal{Z}$. Since $\mathcal{K}$ and $\mathcal{P}$ preserve weak equivalences, they induce functors on the homotopy category. Using this and the fact that v is a weak equivalence for a special Γ-category, we get a map

$$R\colon [\mathcal{WX},\mathcal{Z}] \longrightarrow [\mathcal{KPX},\mathcal{Z}]$$

as follows: Given f in $[\mathcal{WX},\mathcal{Z}]$, the map Rf in $[\mathcal{KPX},\mathcal{Z}]$ is the composite

$$\mathcal{KPX} \xrightarrow{\mathcal{KP}\omega^{-1}} \mathcal{KPWX} \xrightarrow{\mathcal{KP}f} \mathcal{KPZ} \xrightarrow{v^{-1}} \mathcal{WZ} \xrightarrow{\omega} \mathcal{Z}.$$

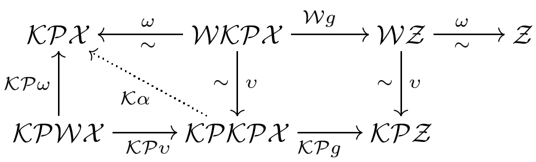
To see that the composite map on $[\mathcal{WX},\mathcal{Z}]$ is the identity, consider the following diagram,



which commutes by naturality. We see that $\mathcal{W}\omega$ is a weak equivalence (as marked) by the two-out-of-three property since ω is always a weak equivalence. The map $R(f)\circ v$ is the composite map in the homotopy category of the part of this diagram starting from the copy of $\mathcal{WX}$ in the first column and traversing maps and inverse maps to $\mathcal{Z}$ by going down, right twice, and then up twice; this agrees with the composite map in the homotopy category obtained by going up and then right twice, $f\circ\omega^{-1}\circ\omega = f$.
On the other hand, starting with g in $[\mathcal{KPX},\mathcal{Z}]$, then

$$R(g\circ v) = \omega\circ v^{-1}\circ \mathcal{KP}(g\circ v\circ\omega^{-1}).$$

The solid arrow part of the diagram



commutes and Lemma 5.7 implies that the whole diagram commutes in the homotopy category. By naturality of ω, the composite $\omega\circ\mathcal{W}g\circ\omega^{-1}$ is g, and it follows that $R(g\circ v)$ is g. □

6. Special Γ-spaces and non-completed E_∞ spaces

This section explores the analogue in simplicial sets of the construction of $\mathcal{P}$ in small categories, which provides a functor E from Γ-spaces to E_∞ spaces over the Barratt-Eccles operad. This section is entirely independent from the rest of the paper and we have written it to be as self-contained as possible without being overly repetitious. We assume familiarity with Γ-spaces, but not with Γ-categories or permutative categories (except where we compare E and $\mathcal{P}$ in Proposition 6.5).

Definition 4.1 describes a category $\mathcal{A}$ whose objects are the sequences of positive integers (including the empty sequence). We think of a positive integer as a finite (unbased) set, and maps between sequences $\vec{m} = (m_1, \dots, m_r)$ and $\vec{n} = (n_1, \dots, n_s)$ are generated by permuting elements in the sequence, maps of finite sets, and partitioning finite sets. For a Γ-space X, let AX be the functor from $\mathcal{A}$ to based simplicial sets with

$$AX(\vec{n}) = X(\mathbf{n}_1) \times \cdots \times X(\mathbf{n}_s)$$

for $s > 0$ and $AX() = *$. In terms of the maps in $\mathcal{A}$, a permutation of sequences induces the corresponding permutation of factors; a map of finite unbased sets $\phi\colon \underline{n} \to \underline{p}$ induces the corresponding map $X(\phi)$ (for the corresponding $\phi\colon \mathbf{n} \to \mathbf{p}$); a partition $\underline{n} = \underline{p}_1 \amalg \cdots \amalg \underline{p}_t$ induces the map

$$X(\mathbf{n}) \longrightarrow X(\mathbf{p}_1) \times \cdots \times X(\mathbf{p}_t)$$

induced by the maps $\mathbf{n} \to \mathbf{p}_i$ that pick out the elements of the subset $\mathbf{p}_i$ and send all the other elements to the basepoint. We consider the homotopy colimit.

Definition 6.1. Let $EX = \operatorname{hocolim}_{\mathcal{A}} AX$.

It is clear from the definition that E preserves weak equivalences. The proof of the remainder of the following theorem is identical to the proof of Theorem 5.3.

Theorem 6.2. *E preserves weak equivalences. If X is a special Γ-space, then the inclusion of $X(\mathbf{1})$ in EX is a weak equivalence.*

Recall that the Barratt-Eccles operad $\mathcal{E}$ has as its n-th simplicial set $\mathcal{E}(n) = NT\Sigma_n$ the nerve of the translation category on the n-th symmetric group Σ_n, with operadic multiplication induced by block sum of permutations. For any permutation σ in Σ_n, we have a functor

$$\sigma\colon \mathcal{A}^{\times n} \longrightarrow \mathcal{A}$$

induced by permutation and concatenation:

$$\sigma(\vec{m}^1, \dots, \vec{m}^n) = (m_1^{\sigma 1}, \dots, m_{r_{\sigma 1}}^{\sigma 1}, m_1^{\sigma 2}, \dots, m_{r_{\sigma n}}^{\sigma n}).$$

Permutation induces a natural transformation

$$AX^{\times n} \longrightarrow AX$$

covering σ; we therefore get an induced map on homotopy colimits

$$\sigma_*\colon (EX)^{\times n} \longrightarrow EX.$$

For any other element $\sigma' \in \Sigma_n$, the permutation $\sigma'\sigma^{-1}$ induces a natural transformation between functors

$$\sigma, \sigma' \colon \mathcal{A}^{\times n} \longrightarrow \mathcal{A},$$

compatible with the natural transformations $AX^{\times n} \to AX$ covering them. These fit together to induce a map

$$\mathcal{E}(n) \times EX^{\times n} \cong NT\Sigma_n \times \mathrm{hocolim}_{\mathcal{A}^{\times n}} AX^{\times n} \longrightarrow EX. \tag{6.3}$$

An easy check of the definitions proves the following proposition, a restatement of Theorem 1.6.

Proposition 6.4. *The maps* (6.3) *define an action of the operad $\mathcal{E}$ on the simplicial set EX. This action is natural in maps of the Γ-space X. Thus, E defines a functor from Γ-spaces to E_∞ spaces over $\mathcal{E}$.*

To compare the functor E with the functor $\mathcal{P}$, recall that the nerve of a permutative category has the natural structure of an $\mathcal{E}$ space with the map $\sigma_* \colon N\mathcal{C}^{\times n} \to N\mathcal{C}$ (for σ in Σ_n) induced by the permutation and the permutative product. In Section 5, we reviewed the map from the homotopy colimit of the nerve to the nerve of the Grothendieck construction, which we can now interpret as a natural transformation $EN \to N\mathcal{P}$. The following proposition is clear from explicit description of the map in that section.

Proposition 6.5. *For a Γ-category $\mathcal{X}$, the canonical map $EN\mathcal{X} \to N\mathcal{P}\mathcal{X}$ is a map of $\mathcal{E}$ spaces and a weak equivalence.*

Next we define the Γ-space version of the functor EX. For this we use the Γ-spaces X_n defined by

$$X_n(\mathbf{m}) = X(\mathbf{nm}),$$

where we use lexicographical ordering to make $\mathbf{nm}$ a functor of $\mathbf{m}$ from $\mathcal{F}$ to $\mathcal{F}$. Taking advantage of the fact that $\mathbf{nm}$ is also a functor of $\mathbf{n}$, the construction $EX_{(-)}$ defines a functor from $\mathcal{F}$ to simplicial sets. However, since we require Γ-spaces to satisfy $X(\mathbf{0}) = *$, we need a reduced version.

Definition 6.6. Let $E^\Gamma X$ be the Γ-space with $E^\Gamma X(\mathbf{n})$ the based homotopy colimit in the category of based simplicial sets

$$E^\Gamma X(\mathbf{n}) = \mathrm{hocolim}^*_{\mathcal{A}} AX_n.$$

The inclusions $\eta_n \colon X_n(\mathbf{1}) \to E^\Gamma X(\mathbf{n})$ now assemble to a map of Γ-spaces $X \to E^\Gamma X$. Since $\mathcal{A}$ has an initial object (), the nerve $N\mathcal{A}$ is contractible. The map

$$EX_n = \mathrm{hocolim}_{\mathcal{A}} AX_n \longrightarrow (\mathrm{hocolim}_{\mathcal{A}} AX_n)/N\mathcal{A} = \mathrm{hocolim}^*_{\mathcal{A}} AX_n = E^\Gamma X(\mathbf{n})$$

is therefore a weak equivalence. Applying Theorem 6.2 objectwise to the map $X \to E^\Gamma X$, we get the following theorem.

Theorem 6.7. *E^Γ preserves weak equivalences. If X is a special Γ-space, then the natural map $X \to E^\Gamma X$ is a weak equivalence.*

We prove the following theorem at the end of the section.

Theorem 6.8. *For a Γ-space X, $E^\Gamma X$ is a special Γ-space.*

Finally, we need one further variant of this construction. Let AEX be the functor from $\mathcal{A}$ to simplicial sets with

$$AEX(\vec{n}) = EX_{n_1} \times \cdots \times EX_{n_s}$$

and $AE() = EX_0 = E*$: Although $EX_{(-)}$ is not a Γ-space, it is an $\mathcal{F}$-space (functor from $\mathcal{F}$ to simplicial sets), and this is all that is needed for the construction of the functor AEX. Let E^2X be the simplicial set

$$E^2X = \operatorname{hocolim}_{\mathcal{A}} AEX$$

(homotopy colimit in the category of unbased simplicial sets). The map of $\mathcal{F}$-spaces $EX_{(-)} \to E^\Gamma X(-)$ induces a weak equivalence $AEX \to AE^\Gamma X$ and a weak equivalence $E^2X \to E(E^\Gamma X)$.
The advantage of E^2X over $E(E^\Gamma X)$ is that we can construct a map $E^2X \to EX$ as follows. For each $\vec{m}$ in $\mathcal{A}$, we have a map

$$\begin{aligned} AEX(\vec{m}) = EX_{m_1} \times \cdots \times EX_{m_r} &\cong \operatorname{hocolim}_{\mathcal{A}^{\times r}}(AX_{m_1} \times \cdots \times AX_{m_r}) \\ &\longrightarrow \operatorname{hocolim}_{\mathcal{A}} AX = EX \end{aligned}$$

induced by the functor $\rho_{\vec{m}} \colon \mathcal{A}^{\times r} \to \mathcal{A}$, defined by

$$\rho_{\vec{m}} \colon (\vec{n}_1, \ldots, \vec{n}_r) \mapsto (m_1 n_{1,1}, \ldots, m_1 n_{1,s_1}, m_2 n_{2,1}, \ldots, m_r n_{r,s_r})$$

(where $\vec{n}_i = (n_{i,1}, \ldots, n_{i,s_i})$), together with the canonical isomorphism

$$AX_{m_1}(\vec{n}_1) \times \cdots \times AX_{m_r}(\vec{n}_r) \cong AX(\rho_{\vec{m}}(\vec{n}_1, \ldots, \vec{n}_r))$$

covering $\rho_{\vec{m}}$. These maps are compatible with maps $\vec{m}$ in $\mathcal{A}$, and so induce a map $\alpha \colon E^2X \to EX$. The technical fact about this map we need is the following lemma, which is an easy check of the construction.

Lemma 6.9. *The diagram*

$$\begin{array}{ccc} EX & \xrightarrow{\ \eta\ } & E^2X \\ {\scriptstyle E\eta}\downarrow & \searrow^{\mathrm{id}} & \downarrow{\scriptstyle \alpha} \\ E^2X & \xrightarrow[\ \alpha\ ]{} & EX \end{array}$$

commutes where η is induced by the inclusion of EX as $AEX(1)$ and $E\eta$ is induced by the inclusion of AX in AEX.

Applying the lemma to X_n, we get a commuting diagram of $\mathcal{F}$-spaces. We can turn this into a diagram of Γ-spaces by taking the quotient by $EX_0 = E*$ or $E^2X_0 = E^2*$ at each spot. We then get a commutative diagram of Γ-spaces

$$\begin{array}{ccc} E^\Gamma X & \xrightarrow{\ \eta\ } & E^2X_{(-)}/E^2* \\ {\scriptstyle E\eta}\downarrow & \searrow^{\mathrm{id}} & \downarrow{\scriptstyle \alpha} \\ E^2X_{(-)}/E^2* & \xrightarrow[\ \alpha\ ]{} & E^\Gamma X. \end{array}$$

We note that E^2* is contractible, and since $E^\Gamma X$ is special, η is weak equivalence. It follows that all maps in the diagram are weak equivalences. Since both

$$\eta\colon E^\Gamma X \longrightarrow E^\Gamma E^\Gamma X \qquad \text{and} \qquad E^\Gamma \eta\colon E^\Gamma X \longrightarrow E^\Gamma E^\Gamma X$$

factor through the corresponding map $E^\Gamma X \to E^2 X/E^2*$, we get the following proposition.

Proposition 6.10. *The maps η and $E^\Gamma\eta$ from $E^\Gamma X$ to $E^\Gamma E^\Gamma X$ coincide in the strict homotopy category of Γ-spaces, i.e., the homotopy category obtained by formally inverting the objectwise weak equivalences.*

We use this observation to prove the following theorem, which together with Theorems 6.7 and 6.8 imply Theorem 1.5.

Theorem 6.11. *For any Γ-space X, $\eta\colon X \to E^\Gamma X$ is a stable equivalence. Moreover η is the initial map from X to a special Γ-space in the strict homotopy category of Γ-spaces.*

Proof. We need to show that for any special Γ-space Z, the map η induces a bijection $[E^\Gamma X, Z] \to [X, Z]$ where $[-,-]$ denotes maps in the strict homotopy category of Γ-spaces. Since E^Γ preserves weak equivalences, it induces a functor on the strict homotopy category. Given a map g in $[X,Z]$, $E^\Gamma g$ is a map in $[E^\Gamma X, E^\Gamma Z]$, and since $\eta\colon Z \to EZ$ is a weak equivalence, we can compose with the map η^{-1} in the strict homotopy category to get an element $Rg = \eta^{-1} \circ E^\Gamma g$ in $[E^\Gamma X, Z]$. By naturality of η, R is a retraction. By examination of the solid arrow commuting diagram

$$\begin{array}{ccccc}
X & \xrightarrow{\ \eta\ } & E^\Gamma X & \xrightarrow{\ g\ } & Z \\
 & {\scriptstyle \mathrm{id}} \nearrow & \sim \downarrow {\scriptstyle \eta} & & \sim \downarrow {\scriptstyle \eta} \\
E^\Gamma X & \xrightarrow[E^\Gamma \eta]{} & E^\Gamma E^\Gamma X & \xrightarrow[E^\Gamma g]{} & E^\Gamma Z
\end{array}$$

and applying the previous proposition, we see that R is a bijection. □

The previous theorem also provides the final piece for the proof of Theorem 1.9.

Proof of Theorem 1.9. The equivalence of (iii) and (iv) is Theorem 1.4 proved in the last section. The previous theorem proves the equivalence of (ii) and (iii), and [12, 1.8] (and the argument for [9, 1.1]) prove the equivalence of (i) and (iii). □

We close with the proof of Theorem 6.8. We thank Irene Sami for help putting together this argument.

Proof of Theorem 6.8. It suffices to show that for every $j > 0$, the map

$$EX_{j+1} \longrightarrow EX_j \times EX \tag{6.12}$$

is a weak equivalence. Using EX_j in place of $E^\Gamma X(\mathbf{j})$ has the advantage that we can write $EX_j \times EX$ as a homotopy colimit:

$$EX_j \times EX \cong \mathrm{hocolim}_{\mathcal{A}\times\mathcal{A}}(AX_j \times AX).$$

For clarity in formulas that follow, we will use brackets $[m]$ rather than bold $\mathbf{m}$ to denote finite based sets.
The map (6.12) is induced by the diagonal functor $\mathcal{A} \to \mathcal{A}\times\mathcal{A}$ and the natural transformation

$$AX_{j+1}(\vec{m}) \longrightarrow AX_j(\vec{m}) \times AX(\vec{m}).$$

We get a map

$$EX_j \times EX \longrightarrow EX_{j+1} \tag{6.13}$$

induced by the concatenation functor $\mathcal{A}\times\mathcal{A} \to \mathcal{A}$ and the natural transformation

$$AX_j(\vec{m}) \times AX(\vec{n}) \longrightarrow AX_{j+1}(\vec{m} \,\Box\, \vec{n})$$

(where $\Box$ denotes concatenation), sending

$$X([jm_1]) \times \cdots \times X([jm_r]) \longrightarrow X([(j+1)m_1]) \times \cdots \times X([(j+1)m_r])$$

by the map induced by the inclusion of $[j]$ in $[j+1]$, and the map

$$X([n_1]) \times \cdots \times X([n_s]) \longrightarrow X([(j+1)n_1]) \times \cdots \times X([(j+1)n_s])$$

induced by including the non-basepoint element 1 of $[1]$ as the element $j+1$ of $[j+1]$. We show that (6.12) and 6.13 are inverse generalized simplicial homotopy equivalences.
First we show that the composite on E_{j+1} is (generalized simplicial) homotopic to the identity. We denote the composite on E_{j+1} as (D,d). It is induced by the functor $D\colon \mathcal{A} \to \mathcal{A}$ that sends $\vec{m}$ to the concatenation $\vec{m} \,\Box\, \vec{m}$ and the natural transformation

$$\begin{aligned} d\colon X_{j+1}(m_i) &= \\ & X([(j+1)m_i]) \longrightarrow X([(j+1)m_i]) \times X([(j+1)m_i]) = X_{j+1}(m_i, m_i) \end{aligned}$$

induced in the first factor by sending the element $j+1$ of $[j+1]$ to the basepoint and induced in the second factor by sending the elements $1, \ldots, j$ of $[j+1]$ to the basepoint.
We construct a new map (H,h) from E_{n+1} to itself and simplicial homotopies from (H,h) to (D,d) and from (H,h) to the identity as follows. Let H be the functor $\mathcal{A} \to \mathcal{A}$ that sends $(m_1, \ldots, m_r)$ to $((j+1)m_1, \ldots, (j+1)m_r)$ and let

$$\begin{aligned} h\colon AX_{j+1}(\vec{m}) &= AX((j+1)m_1, \ldots, (j+1)m_r) \\ &\longrightarrow AX((j+1)^2 m_1, \ldots, (j+1)^2 m_r) = AX_{j+1}(H\vec{m}) \end{aligned}$$

be the natural transformation induced by the diagonal map in $\mathcal{F}$ from $[j+1]$ to $[(j+1)^2]$; then the functor H and natural transformation h induce a map (H,h) from EX_{j+1} to itself.

We have a natural transformation ϕ from H to D formed by concatenation and permutation from the maps

$$((j+1)m_i) \longrightarrow (m_i, m_i)$$

in $\mathcal{A}$ sending collapsing the first j copies of $\underline{m}_i$ to the first $\underline{m}_i$ by the codiagonal map and sending the last copy of $\underline{m}_i$ onto the second $\underline{m}_i$. The composite map

$$AX_{j+1}(\vec{m}) \xrightarrow{h} AX_{j+1}(H\vec{m}) \xrightarrow{AX_{j+1}(\phi)} AX_{j+1}(D\vec{m})$$

is d. Thus, the natural transformation ϕ induces a homotopy between the maps (H,h) and (D,d) on the homotopy colimit E_{j+1}.
Likewise, we have a natural transformation ψ from H to the identity induced by the maps $((j+1)m_i) \to (m_i)$ in $\mathcal{A}$ that collapse the $j+1$ copies of m_i by the codiagonal. Since the composite

$$AX_{j+1}(\vec{m}) \xrightarrow{h} AX_{j+1}(H\vec{m}) \xrightarrow{AX_{j+1}(\psi)} AX_{j+1}(\vec{m})$$

is the identity, it follows that ψ induces a homotopy from H to the identity on EX_{j+1}. This constructs the generalized simplicial homotopy equivalence between the composite map and the identity map on EX_{j+1}.
The argument for the other composite is easier: The composite on $EX_j \times EX$ is induced by the functor D_2 from $\mathcal{A} \times \mathcal{A}$ to itself

$$D_2(\vec{m}, \vec{n}) = (\vec{m} \,\square\, \vec{n}, \vec{m} \,\square\, \vec{n})$$

and the natural transformation

$$d_2 \colon AX_j(\vec{m}) \times AX(\vec{n}) \longrightarrow AX_j(\vec{m} \,\square\, \vec{n}) \times AX(\vec{m} \,\square\, \vec{n})$$

induced on the first factor by the inclusion of $\vec{m}$ in $\vec{m} \,\square\, \vec{n}$ and on the second factor by the inclusion of $\vec{n}$ in $\vec{m} \,\square\, \vec{n}$. Since these maps

$$(\vec{m}, \vec{n}) \longrightarrow (\vec{m} \,\square\, \vec{n}, \vec{m} \,\square\, \vec{n})$$

assemble to a natural transformation in $\mathcal{A} \times \mathcal{A}$ from the identity functor to D_2, they induce a homotopy on $EX_j \times EX$ between the identity and the map induced by D_2, d_2. □

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Special Subvarieties Arising from Families of Cyclic Covers of the Projective Line

Dedicated to Frans Oort on the occasion of his 75th birthday

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Abstract. We consider families of cyclic covers of $\mathbb{P}^1$, where we fix the covering group and the local monodromies and we vary the branch points. We prove that there are precisely twenty such families that give rise to a special subvariety in the moduli space of abelian varieties. Our proof uses techniques in mixed characteristics due to Dwork and Ogus.

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Introduction

According to a conjecture of Coleman, if we fix a genus $g \geqslant 4$ and consider smooth projective curves C over $\mathbb{C}$ of genus g, there should be only finitely many such curves, up to isomorphism, such that $\mathrm{Jac}(C)$ is an abelian variety of CM type. This conjecture is known to be false for $g \in \{4,5,6,7\}$, by virtue of the fact that for these genera there exist special subvarieties $S \subset \mathscr{A}_g$ (also known as subvarieties of Hodge type) of positive dimension that are contained in the (closed) Torelli locus and that meet the open Torelli locus.

All known examples of such special subvarieties S arise from families of cyclic covers of $\mathbb{P}^1$. As input for this we fix integers $m \geqslant 2$ and $N \geqslant 4$, together with an N-tuple $a = (a_1, \ldots, a_N)$; then we consider cyclic covers $C_t \to \mathbb{P}^1$

with covering group $\mathbb{Z}/m\mathbb{Z}$, branch points $t_1, \ldots, t_N$ in $\mathbb{P}^1$, and with local monodromy a_i about t_i. Varying the branch points we obtain an $(N-3)$-dimensional closed subvariety $Z = Z(m, N, a) \subset \mathscr{A}_g$ given by the Jacobians of the curves C_t, and for certain choices of (m, N, a) it can be shown that Z is a special subvariety.

The main purpose of this paper is to give a list of monodromy data (m, N, a) such that $Z(m, N, a)$ is special, and to prove that there are no further such examples.

By construction, the Jacobians J_t come equipped with an action of the group ring $\mathbb{Z}[\mu_m]$. This action defines a special subvariety $S(\mu_m) \subset \mathscr{A}_g$ that contains Z and whose dimension can be easily calculated in terms of the given monodromy data (m, N, a). We always have $N - 3 \leqslant \dim S(\mu_m)$, and if equality holds $Z = S(\mu_m)$ is special. To search for triples (m, N, a) for which $\dim S(\mu_m) = N - 3$ is something that can be done on a computer, and it is therefore surprising that this appears not to have been done until recently. Thus, while examples in genera 4 and 6 have been given by de Jong and Noot in [6]—and in fact, these examples at least go back to Shimura's paper [24]—examples with $g = 5$ and $g = 7$ were found only much later; see Rohde [22]. At any rate, with the help of a computer program we find twenty examples with $\dim S(\mu_m) = N - 3$. The main result of this paper is that this list is complete:

Main theorem. — Consider monodromy data (m, N, a) as above. Then the closed subvariety $Z(m, N, a) \subset \mathscr{A}_{g,\mathbb{C}}$ is special if and only if (m, N, a) is equivalent to one of the twenty triples listed in Table 1.

Note that if $N - 3 < \dim S(\mu_m)$, which means that the inclusion $Z \subset S(\mu_m)$ is strict, Z could a priori still be a special subvariety. The main point of our result is that even in these cases we are able to prove that Z is not special.

To get a feeling for the difficulty of the problem, consider, as an example, the family of (smooth projective) curves of genus 8 given by $y^{10} = x(x-1)(x-t)^2$, where $t \in T = \mathbb{P}^1_{\mathbb{C}} \setminus \{0, 1, \infty\}$ is a parameter. The corresponding family of Jacobians $J \to T$ decomposes, up to isogeny, as a product $J^{\mathrm{old}} \times J^{\mathrm{new}}$ of two abelian fourfolds. (The old part comes from the quotient family $u^5 = x(x-1)(x-t)^2$; the new part is the family of Pryms.) Both J^{old} and J^{new} give rise to a 1-dimensional special subvariety in $\mathscr{A}_4$, and they both admit an action by $\mathbb{Z}[\zeta_5] = \mathbb{Z}[\zeta_{10}]$, with the same multiplicities on the tangent spaces at the origin. A priori it might be true that J^{old} and J^{new} are isogenous, in which case the family $J \to T$ would define a special subvariety in $\mathscr{A}_8$. Our theorem says, in this particular example, that this does not happen.

From the perspective of special points and the André-Oort conjecture, one could state the problem, in the example at hand, as follows. There are infinitely many values for t such that J^{old}_t is of CM type; likewise for J^{new}_t. Do there exist infinitely many t such that J^{old}_t and J^{new}_t are simultaneously of CM type?

Our theorem, combined with a result of Yafaev [25], implies the answer is *no*, at least if we assume the Generalized Riemann Hypothesis. See Corollary 3.7.

Our proof of the main theorem uses techniques from characteristic p and is based on a method that in some particular cases has already been used by de Jong and Noot in [6], Section 5. For a suitable choice of a prime number p, the Jacobians in our family will, at least generically, have ordinary reduction in characteristic p. Moreover, if we assume $Z(m, N, a) \subset \mathscr{A}_g$ to be special then by a result of Noot [18] we can arrange things in such a way that the canonical liftings of these ordinary reductions are again Jacobians. Already over the Witt vectors of length 2 this is a very restrictive condition that, using the results of Dwork and Ogus in [8], can be turned into something computable.
In individual cases (such as the example sketched above, or the examples treated in [6]), these techniques give a rather effective method to prove that some given family of curves does not give rise to a special subvariety in $\mathscr{A}_{g,\mathbb{C}}$. To do this for arbitrary data (m, N, a) is much harder, and some perseverance is required to deal with the combinatorics that is involved. It would be interesting to have a purely Hodge-theoretic proof of the main theorem; as it is, we do not even have a Hodge-theoretic method that works well in individual examples.

Let us give an overview the contents of the individual sections. In Section 1 we quickly review the notion of a special subvariety and we summarize some facts we need. In Section 2 we introduce the families of curves that we want to consider. In Section 3 we discuss the special subvariety $S(\mu_m)$ that contains $Z(m, N, a)$, we give the list of data (m, N, a) for which $Z(m, N, a) = S(\mu_m)$ and we state the main results. Sections 4 and 5 contain the main technical tools for the proof. In Section 4 we discuss how the VHS associated with our family of curves decomposes and we give some results about the monodromy of the summands. In Section 5 we briefly review the techniques of [8] and we give some refinements that we need in order to deal with hyperelliptic families. In Sections 6 and 7, finally, we prove the main theorem, first in the case $N = 4$, then for $N \geqslant 5$. We refer to the beginning of Section 6 for a brief explanation of how the proof works.

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Notation. If x is a real number, $\langle x\rangle = x - \lfloor x\rfloor$ denotes its fractional part. For $a \in \mathbb{Z}/m\mathbb{Z}$ or $a \in \mathbb{Z}$ we denote by $[a]_m$ the unique representative of the class a (resp. the class a mod m) in $\{0,\ldots,m-1\}$.

1. Some preliminaries about special subvarieties

In this section we work over $\mathbb{C}$. We recall the notion of a special subvariety. For further details we refer to [12], where the terminology "subvarieties of Hodge type" was used, and [20].

(1.1) Consider the moduli space $\mathscr{A}_{g,[n]}$ of g-dimensional principally polarized abelian varieties with a level n structure, for some $n \geqslant 3$. We first briefly recall the description of this moduli space as a Shimura variety.
Let $V_{\mathbb{Z}} := \mathbb{Z}^{2g} \subset V := \mathbb{Q}^{2g}$, and let $\Psi\colon V_{\mathbb{Z}} \times V_{\mathbb{Z}} \to \mathbb{Z}$ be the standard symplectic form. Let $G := \mathrm{CSp}(V_{\mathbb{Z}},\Psi)$ be the group of symplectic similitudes. Let $\mathbb{S} := \mathrm{Res}_{\mathbb{C}/\mathbb{R}}\,\mathbb{G}_m$ be the Deligne torus, and let $\mathfrak{H}$ be the space of homomorphisms $h\colon \mathbb{S} \to G_{\mathbb{R}}$ that define a Hodge structure of type $(-1,0)+(0,-1)$ on $V_{\mathbb{Z}}$ for which $\pm(2\pi i)\cdot\Psi$ is a polarization. The pair $(G_{\mathbb{Q}},\mathfrak{H})$ is a Shimura datum, and $\mathscr{A}_g$ can be described as the associated Shimura variety. Concretely, if $K_n := \bigl\{g \in G(\hat{\mathbb{Z}}) \bigm| g \equiv 1 \bmod n\bigr\}$ then $\mathscr{A}_{g,[n]}(\mathbb{C}) \cong G(\mathbb{Q})\backslash\mathfrak{H} \times G(\mathbb{A}_{\mathrm{fin}})/K_n$.
In order to define special subvarieties, consider an algebraic subgroup $H \subset G_{\mathbb{Q}}$ such that

$$Y_H := \bigl\{h \in \mathfrak{H} \bigm| h \text{ factors through } H_{\mathbb{R}}\bigr\}$$

is non-empty. The group $H(\mathbb{R})$ acts on Y_H by conjugation. It can be shown (see [11], Section I.3, or [12], 2.4) that Y_H is a finite union of orbits under $H(\mathbb{R})$. We remark that the condition that Y_H is non-empty imposes strong restrictions on H; it implies, for instance, that H is reductive. If $Y^+ \subset Y_H$ is a connected component and $\eta K_n \in G(\mathbb{A}_{\mathrm{fin}})/K_n$, the image of $Y^+ \times \{\eta K_n\}$ in $\mathscr{A}_{g,[n]}$ is an algebraic subvariety.

(1.2) *Definition.* — A closed irreducible algebraic subvariety $S \subset \mathscr{A}_{g,[n]}$ is called a *special subvariety* if there exist $Y^+ \subset Y_H$ and $\eta K_n \in G(\mathbb{A}_{\mathrm{fin}})/K_n$ as above such that $S(\mathbb{C})$ is the image of $Y^+ \times \{\eta K_n\}$ in $\mathscr{A}_{g,[n]}(\mathbb{C})$.

We refer to [12] and [20] for alternative descriptions and basic properties of special subvarieties.

(1.3) As level structures play no role in what we are doing, we prefer to state our results in terms of the moduli stack $\mathscr{A}_g$. Of course this is a stack, not a variety, but we allow ourselves to abuse terminology and speak of special subvarieties in $\mathscr{A}_g$ (over $\mathbb{C}$), where "special substack" would perhaps be more correct. By definition, then, a special subvariety $S \subset \mathscr{A}_g$ is a closed, reduced and irreducible algebraic substack such that for some (equivalently: any) $n \geqslant 3$ the irreducible components of the inverse image of S under the natural map

$\mathscr{A}_{g,[n]} \to \mathscr{A}_g$ are special. (It is in fact enough to require that some irreducible component is special.)

(1.4) Let $f: X \to T$ be a family of g-dimensional abelian varieties over an irreducible non-singular complex algebraic variety T. Choose a principal polarization λ of X/T, and let $\phi: T \to \mathscr{A}_g$ be the resulting morphism. Whether or not the closure of $\phi(T)$ is a special subvariety of $\mathscr{A}_g$ only depends on the isogeny class of the generic fibre of X/T as an abelian variety over the function field of T. If we replace X/T by an isogenous family or choose a different λ, the morphism ϕ is replaced by some other morphism $\phi': T \to \mathscr{A}_g$, but if $\overline{\phi(T)}$ is special then so is $\overline{\phi'(T)}$. (This is even true without the assumption that λ is a principal polarization, but we shall not need this.) Without ambiguity we may therefore say that X/T is special if $\overline{\phi(T)} \subset \mathscr{A}_g$ is special for some choice of a polarization.

One property we shall use is that if X/T is isogenous to $Y_1 \times Y_2$ and X is special, the factors Y_i are both special. The converse is not true: if Y_1/T and Y_2/T are special, it is not necessarily the case that $(Y_1 \times Y_2)/T$ is special.

(1.5) Let $f: X \to T$ be as in 1.4. Consider the $\mathbb{Q}$-VHS over T with fibres the first cohomology groups $H^1(X_t, \mathbb{Q})$. Let $b \in T(\mathbb{C})$ be a Hodge-generic point for this VHS, and let $M \subset \mathrm{GL}\big(H^1(X_b, \mathbb{Q})\big)$ be the generic Mumford-Tate group of the family. Choose a principal polarization λ of X/T, let $\phi: T \to \mathscr{A}_g$ be the resulting morphism, and write $Z := \overline{\phi(T)}$. Finally, let $S \subset \mathscr{A}_g$ be the smallest special subvariety containing Z.

In order to calculate the dimension of S, it suffices to know the adjoint real group $M^{\mathrm{ad}}_{\mathbb{R}}$. More precisely, if $M^{\mathrm{ad}}_{\mathbb{R}} = Q_1 \times \cdots \times Q_r$ is the decomposition of this group as a product of simple factors, $\dim(S) = \sum_{i=1}^{r} d(Q_i)$, where $d(Q_i)$ is a contribution that only depends on the isomorphism class of the simple group Q_i. The only cases that are relevant for us are that

- $d(Q) = 0$ if Q is anisotropic (compact);
- $d(Q) = pq$ if $Q \cong \mathrm{PSU}(p, q)$;
- $d(Q) = h(h+1)/2$ if $Q \cong \mathrm{PSp}_{2h}$.

2. The setup

In this section, given data (m, N, a) as in the introduction (see 2.1 below), we construct a family of cyclic covers of $\mathbb{P}^1$ over some base scheme T. For later purposes we shall do this over a ring R of finite type over $\mathbb{Z}$.

(2.1) Let m and N be integers with $m \geqslant 2$ and $N \geqslant 2$, and consider an N-tuple of positive integers $a = (a_1, \ldots, a_N)$ such that $\gcd(m, a_1, \ldots, a_N) = 1$. We further require that $a_i \not\equiv 0$ modulo m for all i and $\sum_{i=1}^{N} a_i \equiv 0$ modulo m. The triple (m, N, a) serves as input for our constructions.

We call two such triples (m, N, a) and (m', N', a') equivalent if $m = m'$ and $N = N'$ and if the classes of a and a' in $(\mathbb{Z}/m\mathbb{Z})^N$ are in the same orbit under

$(\mathbb{Z}/m\mathbb{Z})^* \times \mathfrak{S}_N$. Here we let $(\mathbb{Z}/m\mathbb{Z})^*$ act diagonally by multiplication, and the symmetric group $\mathfrak{S}_N$ acts by permutation of the indices.
In what follows we shall usually assume $N \geqslant 4$ but for some arguments it is useful to allow N to be 2 or 3.

(2.2) Let (m, N, a) be a triple as in 2.1. Let R be the ring $\mathbb{Z}[1/m, u]/\Phi_m$ with Φ_m the mth cyclotomic polynomial. We write $\zeta \in R$ for the class of u; it is a root of unity of order m. We embed R into $\mathbb{C}$ by sending ζ to $\exp(2\pi i/m)$. The element ζ defines an isomorphism of R-group schemes $(\mathbb{Z}/m\mathbb{Z})_R \xrightarrow{\sim} \mu_{m,R}$ by $(b \bmod m) \mapsto \zeta^b$.
Let $U \subset (\mathbb{A}^1_R)^N$ be the complement of the big diagonals. In other words, U is the R-scheme of ordered N-tuples $(t_1, \ldots, t_N)$ of distinct points in $\mathbb{A}^1$. Let $B \subset \mathbb{P}^2_U$ be the projective curve over U obtained as the Zariski closure of the affine curve whose fibre over a point $(t_1, \ldots, t_N)$ is given by

$$y^m = (x - t_1)^{a_1} \cdots (x - t_N)^{a_N} = \prod_{i=1}^{N} (x - t_i)^{a_i} \,.$$

We have a μ_m-action on B over U by $\zeta \cdot (x, y) = (x, \zeta \cdot y)$. The rational function x defines a morphism $\pi_B \colon B \to \mathbb{P}^1_U$.
There exist an open subscheme $T \subset U$, a smooth proper curve $f \colon C \to T$ equipped with an action of $\mu_{m,T}$, and a $\mu_{m,T}$-equivariant morphism $\rho \colon C \to B_T$, such that for every point $t \in T$ the morphism on fibres $\rho_t \colon C_t \to B_t$ is a normalization of B_t. Let $\pi := \pi_B \circ \rho \colon C \to \mathbb{P}^1_T$, which is a finite morphism that realizes $\mathbb{P}^1_T$ as the quotient of C by the action of $\mu_{m,T}$. If the context requires it, we include the data (m, N, a) in the notation, writing $C = C(m, N, a)$ for instance. Further we write $J \to T$ for the Jacobian of C over T.
If k is a field and $t = (t_1, \ldots, t_N) \in T(k)$, we can also describe $\pi_t \colon C_t \to \mathbb{P}^1_k$ as the μ_m-cover of $\mathbb{P}^1_k$ with branch points $t_1, \ldots, t_N$ and local monodromy about t_i given by the element $\zeta^{a_i} \in \mu_m$.
The assumption that $\gcd(m, a_1, \ldots, a_N) = 1$ implies that the fibres of $f \colon C \to T$ are geometrically irreducible. Let $r_i := \gcd(m, a_i)$. The Hurwitz formula gives that the fibres have genus

$$g = 1 + \frac{(N-2)m - \sum_{i=1}^{N} r_i}{2}\,, \tag{2.2.1}$$

so we obtain a morphism $\psi \colon T \to \mathscr{M}_g$ over R. Define

$$\phi \colon T \to \mathscr{A}_g \tag{2.2.2}$$

to be the composition of ψ with the Torelli morphism. Up to isomorphism, the morphism ψ, and hence also ϕ, only depends on the equivalence class of the triple (m, N, a) for the equivalence relation defined in 2.1.

(2.3) *Remark.* — For computational purposes we have restricted our attention to the case where all branch points t_i are in $\mathbb{A}^1 \subset \mathbb{P}^1$, and we have not fixed any of these branch points, thereby creating some redundancy and excluding families where one of the branch points is fixed to be the point at ∞. For our main results, the only thing that really matters is the closure of the image of $\phi_{\mathbb{C}}\colon T_{\mathbb{C}} \to \mathscr{A}_{g,\mathbb{C}}$. For instance, while the family of curves $y^{10} = x(x-1)(x-\lambda)$ is not among the families we consider (the point at ∞ being a branch point), the subvariety of $\mathscr{A}_9$ we obtain from this family is the same as the one obtained by taking $m = 10$, with $N = 4$ and $a = (1,1,1,7)$.

(2.4) *Convention.* — In what follows we shall in several steps replace the base scheme T by a subscheme. In such a case, it will be understood that we replace C by its restriction to the new base scheme, and we again write $f\colon C \to T$ for the curve thus obtained. Similarly, we retain the notation for various other objects associated with our family of curves.

(2.5) *Notation.* — Let M be a module over some commutative R-algebra, or a sheaf on some R-scheme, on which the group scheme μ_m acts. For $n \in \mathbb{Z}/m\mathbb{Z}$ we write

$$M_{(n)} := \left\{ x \in M \;\middle|\; \zeta(x) = \zeta^n \cdot x \right\},$$

which in the sheaf case has to be interpreted on the level of local sections. We refer to $M_{(n)}$ as the n-eigenspace of M. We have $M = \oplus_{n\in\mathbb{Z}/m\mathbb{Z}}\, M_{(n)}$.

(2.6) Recall that $r_i = \gcd(m, a_i)$. Consider the μ_m-cover $\pi\colon C_t \to \mathbb{P}^1$ for some $t \in T(k)$, where k is a field. For $i \in \{1,\dots,N\}$ and $n \in \mathbb{Z}$, let

$$l(i,n) := -1 + \left\lceil \frac{r_i - n a_i}{m} \right\rceil = \left\lfloor \frac{-n a_i}{m} \right\rfloor,$$

where the second equality easily follows from the fact that $r_i = \gcd(m, a_i)$. Consider the differential forms

$$\omega_{n,\nu} := y^n \cdot (x-t_1)^\nu \cdot \prod_{i=1}^{N} (x-t_i)^{l(i,n)} \cdot dx\,, \tag{2.6.1}$$

and note that these only depend on the pair $(n \bmod m, \nu)$.

The following result is standard.

(2.7) *Lemma.* — *Let $n \in \mathbb{Z}/m\mathbb{Z}$ with $n \neq 0$. The forms $\omega_{n,\nu}$ for $0 \leqslant \nu \leqslant -2 + \sum_{i=1}^N \left\langle \frac{-na_i}{m} \right\rangle$ are regular 1-forms on C_t and they form a k-basis for $H^0(C_t, \Omega^1)_{(n)}$.*

3. The special subvariety given by the action of the covering group

In this section we work over $\mathbb{C}$ and we fix a triple (m, N, a) as in 2.1 with $N \geqslant 4$. We retain the notation introduced in the previous section, with the convention that all objects are now considered over $\mathbb{C}$ via the chosen embedding $R \hookrightarrow \mathbb{C}$.

(3.1) *Definition.* — We let $Z(m, N, a) \subset \mathscr{A}_{g,\mathbb{C}}$ be the scheme-theoretic (or rather, stack-theoretic) image of the morphism $\phi\colon T \to \mathscr{A}_g$ of (2.2.2).

In other words, $Z(m, N, a)$ is the reduced closed substack of $\mathscr{A}_{g,\mathbb{C}}$ with underlying topological space $\overline{\phi(T)}$. We note that $Z(m, N, a)$ only depends on the equivalence class of (m, N, a) and does not depend on the choice of the open subscheme T in 2.1. The dimension of $Z(m, N, a)$ equals $N - 3$.

(3.2) *Notation.* — It will be convenient to write

$$I(m) := \big[(\mathbb{Z}/m\mathbb{Z}) \setminus \{0 \bmod m\}\big]/\{\pm 1\}\,. \tag{3.2.1}$$

Recall that $\langle x\rangle$ denotes the fractional part of x. For $n \in \mathbb{Z}/m\mathbb{Z}$ we define

$$d_n := \begin{cases} -1 + \sum_{i=1}^{N} \left\langle \frac{-na_i}{m} \right\rangle & \text{if } n \not\equiv 0,\\ 0 & \text{if } n \equiv 0, \end{cases} \tag{3.2.2}$$

which by Lemma 2.7 is the dimension of the (n)-eigenspace of $H^0(C_t, \Omega^1)$, for any $t \in T(\mathbb{C})$.

(3.3) The substack $Z(m, N, a) \subset \mathscr{A}_g$ is contained in a special subvariety $S(\mu_m) \subset \mathscr{A}_g$ determined by the action of $\mathbb{Z}[\mu_m]$ on the relative Jacobian $J \to T$. More precisely, $S(\mu_m)$ is the largest closed, reduced and irreducible substack $S \subset \mathscr{A}_g$ containing $Z(m, N, a)$ such that the homomorphism $\mathbb{Z}[\mu_m] \to \mathrm{End}(J/T)$ induced by the action of μ_m on C/T extends to an action of $\mathbb{Z}[\mu_m]$ on the universal abelian scheme over S.
Choose a base point $b \in T(\mathbb{C})$, and let (J_b, λ) be the corresponding Jacobian with its principal polarization. With $(V_{\mathbb{Z}}, \Psi)$ as in 1.1, choose a symplectic similitude $\sigma\colon H_1(J_b, \mathbb{Z}) \xrightarrow{\sim} V_{\mathbb{Z}}$, where we equip $H_1(J_b, \mathbb{Z})$ with its Riemann form (i.e., the polarization, in the sense of Hodge theory, that corresponds with λ). Via σ, the action of μ_m on J_b induces a structure of a $\mathbb{Q}[\mu_m]$-module on $V = V_{\mathbb{Z}} \otimes \mathbb{Q}$. Consider the algebraic subgroup $H \subset G_{\mathbb{Q}} = \mathrm{CSp}(V, \Psi)$ of $\mathbb{Q}[\mu_m]$-linear symplectic similitudes, i.e., the subgroup given by

$$H := \mathrm{GL}_{\mathbb{Q}[\mu_m]}(V) \cap \mathrm{CSp}(V, \Psi)\,.$$

With notation as in 1.1, the image of $Y_H \subset \mathfrak{H}$ under the map

$$\mathfrak{H} \twoheadrightarrow G(\mathbb{Z})\backslash\mathfrak{H} \cong G(\mathbb{Q})\backslash\mathfrak{H} \times G(\mathbb{A}_{\mathrm{fin}})/G(\hat{\mathbb{Z}}) \cong \mathscr{A}_g(\mathbb{C})$$

is (the set of $\mathbb{C}$-points of) a finite union of algebraic subvarieties of $\mathscr{A}_g$, and the special subvariety $S(\mu_m)$ is the unique irreducible component of this image that contains $Z(m, N, a)$.
The dimension of $S(\mu_m)$ is given by

$$\dim S(\mu_m) = \sum d_{-n} d_n + \begin{cases} \frac{d_k(d_k+1)}{2} & \text{if } m = 2k \text{ is even,} \\ 0 & \text{if } m \text{ is odd,} \end{cases} \tag{3.3.1}$$

where the first sum runs over the pairs $\pm n \in I(m)$ with $2n \not\equiv 0$. See [14], Section 5; see also Remark 4.6 below.
In particular, as $Z(m, N, a) \subset S(\mu_m)$ we have

$$N - 3 \leqslant \dim S(\mu_m)\,. \tag{3.3.2}$$

If equality holds then $Z(m, N, a) = S(\mu_m) \subset \mathscr{A}_g$ is a special subvariety; it then follows that among the Jacobians J_t, for $t \in T(\mathbb{C})$, there are, up to isomorphism, infinitely many Jacobians of CM type. (Here we use that on a special subvariety the CM points lie dense.)

(3.4) *Inventory of examples.* — Table 1 lists twenty triples (m, N, a) with $N \geqslant 4$ for which $N - 3 = \dim S(\mu_m)$, so that $Z(m, N, a) \subset \mathscr{A}_{g,\mathbb{C}}$ is a special subvariety. Our assumption that $N \geqslant 4$ means we are only considering the cases that give rise to a special subvariety of positive dimension.
The first column of the table gives a number that we assign to each example for reference. The examples are sorted first by genus, then by degree of the cover. The second column gives the genus of the curves in the family. In the next three columns we give the data (m, N, a). In most cases there is a unique $a = (a_1, \ldots, a_N)$ in its equivalence class such that $1 \leqslant a_1 \leqslant \cdots \leqslant a_N \leqslant m - 1$ with $\sum a_i = 2m$, and if there is a unique such representative, this is the one we list. If $N = 4$ there are usually two such representatives, the second one being $(m - a_4, m - a_3, m - a_2, m - a_1)$; we list the one which lexicographically comes first. In the last column we give references to places in the literature where the example can be found. Here "S(i)" refers to example (i) in [24], "Mi" refers to example i in the appendix of [17], and dJN(1.3.i) refers to example (1.3.i) in [6]. These examples can also be found in [22]; see 4.8 below.

(3.5) *Remark.* — If we have a triple (m, N, a) as in 2.1 with $N = 3$, the associated subvariety $Z = Z(m, N, a)$ is a special point in $\mathscr{A}_g$.

The following theorem is the main result of this paper. It says that the list of examples in Table 1 is exhaustive.

(3.6) *Theorem. — Consider data (m, N, a) as in* 2.1*, with $N \geqslant 4$. Then $Z(m, N, a) \subset \mathscr{A}_{g,\mathbb{C}}$ is a special subvariety if and only if (m, N, a) is equivalent to one of the twenty examples listed in* Table 1.

By what was explained above, it only remains to be shown that $Z(m, N, a)$ is not special if (m, N, a) is not equivalent to one of the triples in the table. In 4.9

	genus	m	N	a	references
(1)	1	2	4	$(1,1,1,1)$	
(2)	2	2	6	$(1,1,1,1,1,1)$	
(3)	2	3	4	$(1,1,2,2)$	
(4)	2	4	4	$(1,2,2,3)$	
(5)	2	6	4	$(2,3,3,4)$	
(6)	3	3	5	$(1,1,1,1,2)$	S(1), M41
(7)	3	4	4	$(1,1,1,1)$	
(8)	3	4	5	$(1,1,2,2,2)$	S(3), M43
(9)	3	6	4	$(1,3,4,4)$	
(10)	4	3	6	$(1,1,1,1,1,1)$	S(2), M23, dJN(1.3.1)
(11)	4	5	4	$(1,3,3,3)$	S(4), dJN(1.3.2)
(12)	4	6	4	$(1,1,1,3)$	
(13)	4	6	4	$(1,1,2,2)$	
(14)	4	6	5	$(2,2,2,3,3)$	
(15)	5	8	4	$(2,4,5,5)$	
(16)	6	5	5	$(2,2,2,2,2)$	S(5), M44
(17)	6	7	4	$(2,4,4,4)$	S(6), dJN(1.3.3)
(18)	6	10	4	$(3,5,6,6)$	
(19)	7	9	4	$(3,5,5,5)$	
(20)	7	12	4	$(4,6,7,7)$	

Table 1: monodromy data that give rise to a special subvariety

we shall first prove this for $m = 2$. In Section 6 we shall prove the theorem for $N = 4$. The case $N > 4$ is treated in Section 7.
Combining the theorem with the main result of [25] we obtain, for $N = 4$, the following finiteness result for the number of CM fibres.

(3.7) *Corollary. — Assume the Generalized Riemann Hypothesis for CM* *fields. If we have a triple (m,N,a) with $N = 4$ and the equivalence class of this triple is not among the twenty examples listed in* Table 1 *then up to isomorphism there are finitely many Jacobians of CM type in the family $J \to T_{\mathbb{C}}$.*

4. Decomposition of the variation of Hodge structure

In this section we again work over $\mathbb{C}$. We fix a triple (m,N,a) as in 2.1 with $N \geqslant 4$. The corresponding family of curves $C \to T$ gives rise to a variation of Hodge structure over T (over $\mathbb{C}$) on which $\mathbb{Q}[\mu_m]$ acts. We describe the resulting decomposition of the VHS, and we give some results about the monodromy of the summands.

(4.1) Let (m,N,a) be as in 2.1. For $n \in \mathbb{Z}/m\mathbb{Z}$, let $N(n)$ be the number of indices $i \in \{1,\ldots,N\}$ such that $na_i \not\equiv 0$ modulo m. In particular, $N(n) = N$ if $n \in (\mathbb{Z}/m\mathbb{Z})^*$. If $n \neq 0$ then $d_n + d_{-n} = N(n) - 2$.
Let $m' \geqslant 2$ be a divisor of m, say with $m = rm'$. Write $N' := N(r \bmod m)$, and consider the N'-tuple a' in $(\mathbb{Z}/m'\mathbb{Z})^{N'}$ obtained from the N-tuple $(a_1 \bmod m', \ldots, a_N \bmod m')$ by omitting the zero entries. Then (m',N',a') is again a triple as in 2.1; we refer to it as the triple obtained from (m,N,a) by reduction modulo m'.

(4.2) As in 2.2, consider the family of curves $f\colon C \to T$ associated with the triple (m,N,a), where, as in the previous section, we work over $\mathbb{C}$. The cohomology groups $H^1(C_t,\mathbb{Q})$ are the fibres of a polarized $\mathbb{Q}$-VHS with underlying local system $\mathbb{V} := R^1 f_*^{\mathrm{an}}\mathbb{Q}_C$. This $\mathbb{Q}$-VHS comes equipped with an action of the group ring $\mathbb{Q}[\mu_m] = \prod_{d|m} K_d$, where $K_d = \mathbb{Q}[t]/\Phi_d$ is the cyclotomic field of dth roots of unity. Accordingly we have a decomposition of $\mathbb{Q}$-VHS,

$$\mathbb{V} = \oplus_{d|m} \mathbb{V}^{[d]}\,, \tag{4.2.1}$$

where $\mathbb{V}^{[d]}$ is a polarized $\mathbb{Q}$-VHS over T equipped with an action of K_d.

(4.3) Let (m,N,a) be as in 2.1, with $N \geqslant 4$. Let $m' \geqslant 2$ be a proper divisor of m, and let (m',N',a') be the triple obtained from (m,N,a) by reduction modulo m', as in 4.1.
Let $\rho\colon \mathbb{A}^N \to \mathbb{A}^{N'}$ be the projection map, omitting the coordinates x_i for all indices i with $a_i \equiv 0$ modulo m'. Performing the construction of 2.2 we may choose $T = T(m,N,a) \subset \mathbb{A}^N$ and $T' = T(m',N',a') \subset \mathbb{A}^{N'}$ such that ρ maps T to T'. (The map $T \to T'$ is then dominant.) If $f'\colon C' \to T'$ is the family of curves associated with the triple (m',N',a'), the pull-back $\rho^*C' = C' \times_{T'} T$ can be identified with the quotient of C/T modulo the action of $\mu_r \subset \mu_m$, where $r = m/m'$.
Let $\mathbb{V}' = \mathbb{V}(m',N',a')$ be the $\mathbb{Q}$-VHS over T' associated with the triple (m',N',a'). The quotient morphism $C \to \rho^*C'$ over T gives a map $\rho^*\mathbb{V}' \to \mathbb{V}$

and this induces an isomorphism $\rho^*\mathbb{V}' \cong \oplus_{d|m'}\mathbb{V}^{[d]}$. We refer to the sub-$\mathbb{Q}$-VHS $\rho^*\mathbb{V}'$ as the *old part* associated with the divisor m'. The direct summand $\mathbb{V}^{[m]} \subset \mathbb{V}$ is called the *new part*; in the decomposition (4.2.1) it is the only direct summand that is not contained in an old part.

(4.4) *Lemma. — Let the notation and assumptions be as in* 4.3. *Let* $g = g(m,N,a)$ *and* $g' = g(m',N',a')$ *be the respective genera. If* $Z(m,N,a) \subset \mathscr{A}_{g,\mathbb{C}}$ *is a special subvariety then* $Z(m',N',a') \subset \mathscr{A}_{g',\mathbb{C}}$ *is special, too.*

Proof. Suppose $Z(m,N,a)$ is special. Write $J = J(m,N,a) \to T$ and $J' = J(m',N',a') \to T'$ for the respective Jacobians. Then ρ^*J' is an isogeny factor of J. Hence, if $\theta\colon T \to \mathscr{A}_{g',\mathbb{C}}$ is the morphism corresponding to ρ^*J', it follows from 1.4 that the Zariski closure of the image of θ is a special subvariety. But θ is just the composition of the projection $\rho\colon T \to T'$, which is dominant, and the morphism $\phi(m',N',a')\colon T' \to \mathscr{A}_{g',\mathbb{C}}$ associated with the data (m',N',a'). Hence the closure of the image of θ is $Z(m',N',a')$. □

(4.5) With notation as in 2.5, the $\mathbb{C}$-local system $\mathbb{V}_{\mathbb{C}}$ decomposes as $\mathbb{V}_{\mathbb{C}} = \oplus_{n\in\mathbb{Z}/m\mathbb{Z}}\mathbb{V}_{\mathbb{C},(n)}$. The relation with (4.2.1) is that $\mathbb{V}_{\mathbb{C}}^{[d]}$ is the sum of all $\mathbb{V}_{\mathbb{C},(n)}$ with $\mathrm{ord}(n) = d$. We have $V_{\mathbb{C},(0)} = 0$, and for $n \neq 0$ the $\mathbb{C}$-local system $\mathbb{V}_{\mathbb{C},(n)}$ has rank $N(n)-2$, where $N(n)$ is defined as in 4.1. (See also [7], Section 2.)
With real coefficients, and with $I(m)$ as in (3.2.1), we have a decomposition of $\mathbb{R}$-VHS

$$\mathbb{V}_{\mathbb{R}} = \left(\bigoplus_{\pm n\in I(m),2n\not\equiv 0} \mathbb{V}_{\mathbb{R},(\pm n)}\right) \oplus \mathbb{V}_{\mathbb{R},(\frac{m}{2})}\,,$$

where the last summand only occurs if m is even. The decomposition is such that

$$\mathbb{V}_{\mathbb{R},(\pm n)} \otimes_{\mathbb{R}} \mathbb{C} = \mathbb{V}_{\mathbb{C},(n)} \oplus \mathbb{V}_{\mathbb{C},(-n)}$$

and

$$\mathbb{V}_{\mathbb{R},(\frac{m}{2})} \otimes_{\mathbb{R}} \mathbb{C} = \mathbb{V}_{\mathbb{C},(\frac{m}{2})} \quad \text{(for even } m)\,.$$

On the summand $\mathbb{V}_{\mathbb{R},(\pm n)}$ the polarization of the VHS induces a (-1)-hermitian form $\beta_{\pm n}$ of signature (d_n, d_{-n}); see also [7], Corollary (2.21) and (2.23). In case m is even, the polarization induces a symplectic form $\beta_{\frac{m}{2}}$ on $\mathbb{V}_{\mathbb{R},(\frac{m}{2})}$.
As in 3.3 we choose a base point $b \in T(\mathbb{C})$, and a symplectic similitude $\sigma\colon H^1(J_b,\mathbb{Q}) \xrightarrow{\sim} V$. Via this similitude, we identify V with the fibre of $\mathbb{V}$ at b. Correspondingly, we write $V_{\mathbb{R},(\pm n)}$ for the direct summand of $V_{\mathbb{R}}$ that under σ maps to the fibre at b of $\mathbb{V}_{\mathbb{R},(\pm n)}$.
For what follows, it will be convenient to choose the base point b to be a Hodge-generic point with respect to the variation $\mathbb{V}$, so from now on we assume this. Define $\mathrm{Mon} \subset \mathrm{GL}(V)$ and $\mathrm{Hdg} \subset \mathrm{GL}(V)$ to be the algebraic monodromy groups of the $\mathbb{Q}$-local system $\mathbb{V}$ and the Hodge group of the fibre at b, respectively. (Since we have chosen b to be Hodge-generic, Hdg is the generic Hodge group of the VHS.) By [3], Theorem 1, the identity component Mon^0 is a semisimple normal subgroup of Hdg.

(4.6) *Remark.* — The generic Hodge group Hdg is contained in the algebraic group $H := \mathrm{GL}_{\mathbb{Q}[\mu_m]}(V) \cap \mathrm{CSp}(V, \Psi)$ considered in 3.3. Extending scalars to $\mathbb{R}$ we have

$$H_{\mathbb{R}} \cong \left(\prod_{\pm n \in I(m), 2n \not\equiv 0} \mathrm{U}(V_{\mathbb{R},(\pm n)}, \beta_{\pm n}) \right) \times \mathrm{Sp}(V_{\mathbb{R},(\frac{m}{2})}, \beta_{\frac{m}{2}}), \tag{4.6.1}$$

where the symplectic factor only occurs if m is even. Our formula (3.3.1) follows from this together with what was explained in 1.5.

We have $\mathrm{Mon}^0 \subset \mathrm{Hdg} \subset H$. The next proposition gives us information about the projections of the $\mathbb{R}$-group $\mathrm{Mon}^0_{\mathbb{R}}$ onto the various factors in the decomposition (4.6.1).

(4.7) *Proposition.* — (i) *Suppose we have* $\pm n \in I(m)$ *with* $2n \not\equiv 0$ *such that* $d_n \geqslant 1$ *and* $d_{-n} \geqslant 1$. *Then the image of* $\mathrm{Mon}^0_{\mathbb{R}}$ *in* $\mathrm{U}(V_{\mathbb{R},(\pm n)}, \beta_{\pm n})$ *is the special unitary group* $\mathrm{SU}(V_{\mathbb{R},(\pm n)}, \beta_{\pm n})$*, which is isomorphic to* $\mathrm{SU}(d_n, d_{-n})$.
(ii) *If* m *is even, the group* $\mathrm{Mon}^0_{\mathbb{R}}$ *projects surjectively to the symplectic group* $\mathrm{Sp}(V_{\mathbb{R},(\frac{m}{2})}, \beta_{\frac{m}{2}})$*, which is isomorphic to* $\mathrm{Sp}_{2h,\mathbb{R}}$ *with* $h = d_{\frac{m}{2}}$.

Proof. For (i), see Rohde [22], Theorem 5.1.1. For (ii), assume m is even, and let $h := d_{\frac{m}{2}}$. There are then $2h+2$ indices i for which a_i is even, and without loss of generality we may assume these are the indices $i \in \{1, \ldots, 2h+2\}$. With the above notation, $\mathbb{V}_{\mathbb{R},(\frac{m}{2})}$ is the same as $\mathbb{V}^{[2]}_{\mathbb{R}}$, and if we define $\mathrm{Mon}^{[2]} \subset \mathrm{GL}(V^{[2]})$ as the algebraic monodromy group of the $\mathbb{Q}$-local system $\mathbb{V}^{[2]}$ then the image of Mon^0 in $\mathrm{Sp}(V_{\mathbb{R},(\frac{m}{2})}, \beta_{\frac{m}{2}})$ equals $\mathrm{Mon}^{[2],0}_{\mathbb{R}}$. Further, $\mathbb{V}^{[2]}$ is just the local system obtained from the family of hyperelliptic curves $u^2 = (x - t_1) \cdots (x - t_{2h+2})$; cf. 4.3. By [1], Theorem 1 (see also [2]), the connected algebraic monodromy group of this local system is the full symplectic group. □

(4.8) Let (m, N, a) be a triple as in 2.1, with $N \geqslant 4$. Consider the following condition.

(4.8.1) There exists a $\pm n \in I(m)$ with $\{d_n, d_{-n}\} = \{1, N-3\}$, and for all other $\pm n' \in I(m)$, either $d_{n'} = 0$ or $d_{-n'} = 0$.

All examples in Table 1, with the exception of Example 2, satisfy this condition. It has been proven by Rohde in [22] that these nineteen examples are the only examples (up to equivalence) of triples (m, N, a) with $N \geqslant 4$ that satisfy (4.8.1).

(4.9) We now prove Theorem 3.6 for $m = 2$. In this case N is even, $g = (N-2)/2$, and up to equivalence $a = (1, \ldots, 1)$ is the only possibility. Further, $Z(2, N, a) \subset \mathscr{A}_{g,\mathbb{C}}$ is the closure of the hyperelliptic locus in $\mathscr{A}_g$. The assertion is that this is not special for $g \geqslant 3$. This is true because for $g \geqslant 3$ the hyperelliptic locus is not dense in $\mathscr{A}_g$, whereas by (ii) of Proposition 4.7 the generic Hodge group Hdg is the full symplectic group.

In what follows we may therefore assume $m > 2$.

5. Canonical liftings of ordinary Jacobians in positive characteristic

(5.1) We need to recall some definitions and results from the paper [8] by Dwork and Ogus. We first discuss their theory in a general setting. After that, from 5.4 on, we return to the specific families of curves that interest us, and we explain how the results of [8] apply to that situation.
Given an irreducible base scheme T and a smooth projective curve $f\colon C \to T$ we write $\omega_{C/T}$ for $\Omega^1_{C/T}$. Consider the Hodge bundle $\mathbb{E} = \mathbb{E}(C/T) := f_*\omega_{C/T}$, which is a vector bundle on T of rank g, the genus of the fibres. We have a Kodaira-Spencer map KS: $\mathrm{Sym}^2(\mathbb{E}) \to \Omega^1_{T/R}$ and we define

$$\mathscr{K} = \mathscr{K}(C/T) := \mathrm{Ker}\big(\mathrm{Sym}^2(\mathbb{E}) \xrightarrow{\text{mult}} f_*(\omega_{C/T}^{\otimes 2})\big)\,,$$
$$\mathscr{Q} = \mathscr{Q}(C/T) := \mathrm{Coker}\big(f_*(\omega_{C/T}^{\otimes 2})^\vee \xrightarrow{\text{mult}^\vee} \mathrm{Sym}^2(\mathbb{E})^\vee\big)\,,$$

where "mult" is the multiplication map. We remark that $\mathscr{Q}$ can be thought of as the pull-back to T of the normal bundle to the Torelli locus inside $\mathscr{A}_g$. Outside the hyperelliptic locus, mult is surjective and $\mathscr{K}$ is the dual of $\mathscr{Q}$.

(5.2) Let k be an algebraically closed field of characteristic $p > 0$. Consider a smooth projective curve C/k of genus g such that its Jacobian J is ordinary. Let λ be the natural principal polarization of J. By Serre-Tate theory (see [9] or [10], Chap. 5) we have a canonical lifting of (J, λ) to a principally polarized abelian variety $(J^{\mathrm{can}}, \lambda^{\mathrm{can}})$ over the ring of Witt-vectors $W(k)$. In general, for $g \geqslant 4$ this canonical lifting is not the Jacobian of a curve over $W(k)$. More precisely, Dwork and Ogus show that in general not even the canonical lifting over $W_2(k)$, the Witt-vectors of length 2, is again a Jacobian.
Following [8] we call the ordinary curve C/k *pre-W_2-canonical* if there exists a smooth projective curve Y over $W_2(k)$ such that $(J^{\mathrm{can}}, \lambda^{\mathrm{can}})$ over $W_2(k)$ is isomorphic, as a principally polarized abelian variety, to the Jacobian of Y.
The main advantage of working modulo p^2 is that in this case there is a natural class $\beta_{C/k}$ in $\mathscr{Q}(C/k)$ that vanishes if and only if C/k is pre-W_2-canonical; see [8], Prop. (2.4). This invariant $\beta_{C/k}$ cannot be defined in a family of curves (in a sense that can be made precise, see [8], § 3), but its Frobenius pullback can, as we shall discuss next.
Let T be a smooth k-scheme, and let $F_T\colon T \to T$ be its absolute Frobenius endomorphism. Consider a smooth projective curve $f\colon C \to T$ such that all fibres C_t are ordinary. This assumption permits us to view the inverse Cartier operator as an $\mathscr{O}_T$-linear homomorphism

$$\gamma\colon F_T^*\mathbb{E} \to \mathbb{E}\,,$$

with $\mathbb{E} = \mathbb{E}(C/T)$ the Hodge bundle. This map γ is the inverse transpose of the Frobenius action on $R^1 f_* \mathscr{O}_C$.
Dwork and Ogus define a global section $\tilde{\beta}_{C/T}$ of $F_T^* \mathscr{Q}(C/T)$ such that for any $t \in T(k)$ the value of $\tilde{\beta}_{C/T}$ at t is $F_k^*(\beta_{C_t/k})$. See [8], Prop. 2.7.
The sheaf $F_T^* \mathscr{Q}(C/T)$ comes equipped with a canonical flat connection

$$\nabla\colon F_T^* \mathscr{Q}(C/T) \to F_T^* \mathscr{Q}(C/T) \otimes \Omega^1_{T/k}\,.$$

In particular, still with T smooth over k, if C_t/k is pre-W_2-canonical for all $t \in T(k)$, the section $\tilde{\beta}_{C/T}$ is zero, so certainly $\nabla \tilde{\beta}_{C/T} = 0$. One of the main points of [8], then, is that $\nabla \tilde{\beta}_{C/T}$ can be calculated explicitly. The result is easiest to state under the additional hypothesis that the fibres C_t are not hyperelliptic. We note that this assumption is not always satisfied in the situation we want to consider. In Prop. 5.8 we shall give a modified version of the next result that also works for hyperelliptic families.
If the C_t are not hyperelliptic, the multiplication map $\mathrm{Sym}^2(\mathbb{E}) \to f_*(\omega^{\otimes 2})$ is surjective, so, with notation as introduced in 5.1, $\tilde{\beta}_{C/T}$ can be viewed as an $\mathscr{O}_T$-linear map $F_T^* \mathscr{K} \to \mathscr{O}_T$.
The following result is [8], Prop. 3.2. (In [8] the result is stated under some versality assumption on the family C/T but one easily verifies that their Prop. 3.2 is true without this assumption.)

(5.3) *Proposition (Dwork-Ogus). — With assumptions and notation as above, and assuming the curves C_t to be non-hyperelliptic, $-\nabla(\tilde{\beta}_{C/T})\colon F_T^* \mathscr{K} \to \Omega^1_{T/k}$ is equal to the composition*

$$F_T^* \mathscr{K} \xhookrightarrow{\text{incl}} F_T^* \mathrm{Sym}^2(\mathbb{E}) \xrightarrow{\mathrm{Sym}^2(\gamma)} \mathrm{Sym}^2(\mathbb{E}) \xrightarrow{\mathrm{KS}} \Omega^1_{T/k}\,.$$

(5.4) *Assumptions.* — In the rest of this section we fix data (m, N, a) as in 2.1 with $m > 2$ and $N \geqslant 4$, and we consider the family of curves $f\colon C \to T$ as constructed in 2.2. We assume that (m, N, a) is not equivalent to one of the triples listed in Table 1. We further assume that the closed subvariety $Z(m, N, a) \subset \mathscr{A}_{g,\mathbb{C}}$ is a special subvariety; our aim is to derive a contradiction. Without loss of generality we may suppose (m, N, a) is minimal with respect to the above assumptions, by which we mean that there is no triple (m', N', a') that satisfies our assumptions and for which we have $4 \leqslant N' < N$ or $N' = N$ and $2 \leqslant m' < m$. In particular, it follows from Lemma 4.4 that if m' is a proper divisor of m and (m', N', a') is obtained from (m, N, a) by reduction modulo m', as in 4.3, either $N' \leqslant 3$ or (m', N', a') is equivalent to one of the twenty triples listed in Table 1.

(5.5) *Lemma.* — (i) *The subsheaf* $f_*(\omega_{C/T}^{\otimes 2})_{(0)}$ *of* μ_m*-invariant sections of* $f_*(\omega_{C/T}^{\otimes 2})$ *is a locally free* $\mathscr{O}_T$*-module of rank* $N-3$.
(ii) *The Kodaira-Spencer morphism* $\mathrm{KS}\colon \mathrm{Sym}^2(\mathbb{E}) \to \Omega^1_{T/R}$ *factors over the composite map*

$$\mathrm{Sym}^2(\mathbb{E}) \xrightarrow{\mathrm{pr}} \mathrm{Sym}^2(\mathbb{E})_{(0)} \xrightarrow{\mathrm{mult}} f_*(\omega_{C/T}^{\otimes 2})_{(0)}$$

and the induced map $\mathrm{KS}_{(0)}\colon f_*(\omega_{C/T}^{\otimes 2})_{(0)} \to \Omega^1_{T/R}$ *is a fibrewise injective homomorphism of vector bundles.*

Proof. (i) By a result of Chevalley and Weil in [5], for every $t \in T(\mathbb{C})$ the subspace of μ_m-invariants in $H^0(C_t, \Omega^{\otimes 2})$ has dimension $N-3$.
(ii) The fibre of $\mathrm{Sym}^2(\mathbb{E})_{(0)}$ at a point t is dual to the space $H^1(C_t, \Theta)_{(0)}$, which parametrizes the deformations of C_t for which the μ_m-action deforms along. Since we have a μ_m-action on the whole family C/T, the Kodaira-Spencer map factors through the projection $\mathrm{Sym}^2(\mathbb{E}) \to \mathrm{Sym}^2(\mathbb{E})_{(0)}$. For any family of curves it also factors through the multiplication map $\mathrm{Sym}^2(\mathbb{E}) \to f_*(\omega_{C/S}^{\otimes 2})$; hence KS factors through $f_*(\omega_{C/T}^{\otimes 2})_{(0)}$. The last assertion of (ii) just says that at any $t \in T(k)$ our family is complete in the sense of deformation theory: if $D \to \mathrm{Spec}\big(k[\epsilon]\big)$ is a first-order deformation of C_t with its μ_m-action, $D/k[\epsilon]$ can be obtained by pull-back from our family. This is clear, as the quotient D/μ_m is isomorphic to $\mathbb{P}^1_{k[\epsilon]}$. ☐

(5.6) *Lemma.* — *There exists a prime number* p *with* $p \equiv 1$ *modulo* m *and, for* $\mathfrak{p}$ *a prime of* $R = \mathbb{Z}[1/m, u]/\Phi_m$ *above* p*, a dense open subset* U *of* $T_0 := T \otimes_R (R/\mathfrak{p})$*, such that for any algebraically closed field* k *of characteristic* p *and any* $t \in U(k)$ *the curve* C_t *is ordinary and the Jacobian* J_t *is pre-*W_2*-canonical.*

Proof. Let p be any prime number with $p \equiv 1 \bmod m$. Note that in this case $R/\mathfrak{p} = \mathbb{F}_p$ for any prime $\mathfrak{p} \subset R$ above p. We write $T \otimes \mathbb{F}_p$ for $T \otimes_R (R/\mathfrak{p})$. By [4], Prop. 7.4, there is a Zariski open $U \subset T \otimes \mathbb{F}_p$ such that C_t is ordinary for all $t \in U(k)$. On the other hand, by a theorem of Noot [18], [19], in the slightly more precise formulation of [13], Thm. 4.2, the assumption that $Z = Z(m,N,a)$ is special implies that for p large enough and $t \in T_0(k)$ any ordinary point, the canonical lifting of J_t gives a $W(k)$-valued point of Z. In particular, J_t is then pre-W_2-canonical. ☐

(5.7) For most choices of (m,N,a) the general member in our family of curves $C \to T$ is not hyperelliptic. In this case we may, and will, choose p and U in Lemma 5.6 such that the curves C_t with $t \in U(k)$ are non-hyperelliptic.
It may happen, however, that $Z(m,N,a)$ is fully contained in the hyperelliptic locus, in which case we call (m,N,a) a hyperelliptic triple. This occurs, for instance, if $m = 2m'$ is even and a is of the form $(a_1, a_2, m', \ldots, m')$, or if $N = 4$ and $a = (1,1,m-1,m-1)$. In such a case we will just choose p and U as in Lemma 5.6.

The following variant of Prop. 5.3 is the essential tool in our proof of Theorem 3.6. Let p and U be chosen as above, and let $C_U \to U$ be the restriction of C/T to U. With notation as in 2.5 and 5.1 we have eigenspace decompositions $\mathscr{Q}(C_U/U) = \oplus_{n\in\mathbb{Z}/m\mathbb{Z}}\, \mathscr{Q}_{(n)}$; likewise for other $\mathscr{O}_U[\mu_m]$-modules such as $\mathscr{K}(C_U/U)$ and $\mathbb{E}_U = \mathbb{E}(C_U/U)$. Accordingly we can write $\tilde{\beta}_{C_U/U} = \sum_n \tilde{\beta}_{(n)}$, with $\tilde{\beta}_{(n)}$ a section of $F_U^*\mathscr{Q}_{(n)}$.

(5.8) *Proposition. — With assumptions and notation as in* 5.4 *and* 5.7*, the composite map*
(5.8.1)

$$F_U^*\mathscr{K}_{(0)} \xhookrightarrow{\text{incl}} F_U^*\mathrm{Sym}^2(\mathbb{E}_U)_{(0)} \xrightarrow{\mathrm{Sym}^2(\gamma)} \mathrm{Sym}^2(\mathbb{E}_U)_{(0)} \xrightarrow{\mathrm{mult}_{(0)}} f_*(\omega_{C/U}^{\otimes 2})_{(0)}$$

is zero.

Proof. If (m,N,a) is non-hyperelliptic this is immediate from Prop. 5.3 together with (ii) of Lemma 5.5. So from now on we may assume that $Z(m,N,a)$ is contained in the hyperelliptic locus. Let $\iota \in \mathrm{Aut}(C_U/U)$ be the hyperelliptic involution. We remark that ι may or may not be contained in the subgroup $\mu_m \subset \mathrm{Aut}(C_U/U)$; by inspection of the hyperelliptic examples mentioned in 5.7 we see that both cases occur.
Let $\omega = \Omega^1_{C_U/U}$. In the hyperelliptic case the multiplication map $\mathrm{Sym}^2(\mathbb{E}_U) \to f_*(\omega^{\otimes 2})$ is no longer surjective. However, if we denote the invariants under the action of ι by a subscript "even",

$$\mathrm{mult}_{(\mathrm{even})}\colon \mathrm{Sym}^2(\mathbb{E}_U)_{(\mathrm{even})} \to f_*(\omega^{\otimes 2})_{(\mathrm{even})}$$

is again surjective; see for instance [21], Lemmas 2.12 and 2.13. The assumption that $Z(m,N,a)$ is fully contained in the hyperelliptic locus implies that $f_*(\omega^{\otimes 2})_{(0)} \subset f_*(\omega^{\otimes 2})_{(\mathrm{even})}$. Hence also $\mathrm{mult}_{(0)}$ is surjective, and we may view $\tilde{\beta}_{(0)}$ as an $\mathscr{O}_U$-linear map $F_U^*\mathscr{K}_{(0)} \to \mathscr{O}_U$.
Our assumptions imply that $\tilde{\beta}_{(0)}$, hence also $\nabla\tilde{\beta}_{(0)}$, is zero, so all that remains to be checked is that for the 0-component the analogue of Prop. 5.3 holds. For this we can follow the proof of [8], Prop. 3.2: The proof that loc. cit. diagram (3.2.9) is commutative does not use the assumption that the curves are non-hyperelliptic and therefore goes through in the hyperelliptic case. Moreover, in the notation of that proof, we can choose the lifted family $\boldsymbol{Y}/\boldsymbol{T}$ (where Y/T is our C_U/U) such that it has an action of μ_m. Taking 0-components in diagram (3.2.9) then gives that $-\nabla\tilde{\beta}_{(0)}$ equals the composition of (5.8.1) and $\mathrm{KS}_{(0)}$, and by (ii) of Lemma 5.5 we conclude that the map (5.8.1) is zero. □

(5.9) *Lemma. — Write $q = (p-1)/m$. Let $n \in \mathbb{Z}/m\mathbb{Z}$, and let $A = A_n(t) \in \mathrm{GL}_{d_n}(\mathscr{O}_U)$ be the matrix of the Cartier operator $\gamma^{-1}\colon \mathbb{E}_{U,(n)} \to F_U^*\mathbb{E}_{U,(n)}$ with regard to the frames*

$$\omega_{n,0},\ldots,\omega_{n,d_n-1}\,, \quad \textit{respectively} \quad \omega_{n,0}\otimes 1,\ldots,\omega_{n,d_n-1}\otimes 1\,.$$

Then the matrix coefficient $A_{\rho,\sigma}$*, for* ρ, $\sigma \in \{0,\ldots,d_n-1\}$*, equals*

$$(5.9.1)\qquad (-1)^{\Sigma}\cdot \sum_{j_1+\cdots+j_N=\Sigma} \binom{q\cdot[-na_1]_m}{j_1}\cdots\binom{q\cdot[-na_N]_m}{j_N}\cdot t_1^{j_1}\cdots t_N^{j_N}\,,$$

where $\Sigma = (d_n-\sigma)(p-1)+(\rho-\sigma)$.

Proof. This is the dual version of [4], Lemma 5.1, part (i). □

We remark that the result of Bouw in [4] is valid in a more general context. She uses this to prove the existence of cyclic covers whose p-rank reaches a natural upper bound imposed by the local monodromy data; see [4], Thm. 6.1.

6. Proof of the main result: four branch points

In this section we prove Theorem 3.6 in the case $N = 4$. Let us first try to explain the idea of the argument, by way of guide for the reader.
Assume we have a triple (m,N,a) that is not one of the twenty examples in Table 1 but such that $Z(m,N,a)$ is special. We want to show that this is impossible. We have the family of curves $C \to T$ over a ring R of finite type over $\mathbb{Z}$; we then consider the reduction modulo p, with p chosen as in 5.7. The nontrivial information we have, exploiting the assumption that $Z(m,N,a)$ is special, is that this gives a family of ordinary Jacobians in characteristic p such that the canonical liftings over $W_2(k)$ are again Jacobians. In Prop. 5.8 we have translated this, based on the theory in [8], into the vanishing of a certain abstractly defined map. Lemma 5.9 enables us to calculate this map explicitly. To apply this, we need a differential form that gives us an element in the source of the map (5.8.1); we write down such a form in 6.2 below. The fact that the image of this element is zero then gives us a polynomial identity (6.2.1). By some combinatorial arguments we then show that this identity cannot hold if (m,N,a) is not equivalent to one of the twenty special triples in Table 1.

(6.1) We retain the assumptions made in 5.4. In addition we assume $N = 4$. Let

$$\mathscr{D}(m,a) := \bigl\{\pm n \in I(m) \bigm| d_n = d_{-n} = 1\bigr\}\,.$$

(Here $I(m)$ is as defined in (3.2.1) and d_n is given by (3.2.2). Though not indicated in the notation, d_n depends on a.)
If $\pm n \in \mathscr{D}(m,a)$, the equalities $d_n = d_{-n} = 1$ imply that $na_i \not\equiv 0$ modulo m for all $i \in \{1,\ldots,4\}$. Hence,

$$(6.1.1)\qquad [-na_i]_m = m - [na_i]_m \quad \text{for all } i, \qquad \text{and} \qquad \sum_{i=1}^{4} [-na_i]_m = 2m\,,$$

where we recall that $[b]_m$ denotes the representative of the class $(b \bmod m)$ in $\{0,1,\ldots,m-1\}$.

We first observe that $\dim S(\mu_m) > 1$. Indeed, if $\dim S(\mu_m) = 1$ then (4.8.1) holds, and by the results of [22], Chapter 6, (m, N, a) is one of the triples in Table 1, which contradicts our assumptions.
For $n \in \mathbb{Z}/m\mathbb{Z}$ we have $d_n + d_{-n} \leqslant 2$, and if m is even then $d_{\frac{m}{2}} \leqslant 1$. The inequality $\dim S(\mu_m) > 1$ is therefore equivalent to the fact that $\#\mathscr{D}(m, a) \geqslant 2$. Choose two distinct pairs $\pm n$ and $\pm n'$ in $\mathscr{D}(m, a)$. Note that if m is even, we may have $n = -n$ or $n' = -n'$.

(6.2) Choose p and U as in Lemma 5.6, where we may further assume that the curves C_t for $t \in U(k)$ are either all non-hyperelliptic or all hyperelliptic. We keep the notation introduced in the previous section; in particular we recall that $\mathscr{K}(C_U/U) = \oplus_{n\in\mathbb{Z}/m\mathbb{Z}} \mathscr{K}_{(n)}$.
It follows from (6.1.1) and the definition of the forms $\omega_{n,\nu}$ in (2.6.1) that

$$\eta := \omega_{n,0} \otimes \omega_{-n,0} - \omega_{n',0} \otimes \omega_{-n',0}$$

is a section of $\mathscr{K}_{(0)}$. For $\nu \in \{\pm n, \pm n'\}$ the matrix $A_\nu = A_\nu(t)$ of Lemma 5.9 is a polynomial in $\mathbb{F}_p[t_1, \ldots, t_4]$. As the Jacobians of the curves C_t for $t \in U(k)$ are ordinary, the Cartier operator γ^{-1} in Lemma 5.9 is an isomorphism of vector bundles, so $A_\nu(t)$ is invertible as a section of $\mathscr{O}_U$. Because $\omega_{n,0} \cdot \omega_{-n,0} = \omega_{n',0} \cdot \omega_{-n',0}$ is a non-zero section of $f_*(\omega^{\otimes 2})$, it follows from Prop. 5.8 that

$$A_n \cdot A_{-n} = A_{n'} \cdot A_{-n'} \tag{6.2.1}$$

as polynomials.
Define $B_\nu := A_\nu|_{t_1=0}$, the polynomial obtained from A_ν by substituting $t_1 = 0$. Explicitly,
(6.2.2)

$$B_\nu = (-1)^{p-1} \cdot \sum_{j_2+j_3+j_4=p-1} \binom{q \cdot [-\nu a_2]_m}{j_2} \cdots \binom{q \cdot [-\nu a_4]_m}{j_4} \cdot t_2^{j_2} t_3^{j_3} t_4^{j_4} \,.$$

Fix an index $\iota \in \{2, 3, 4\}$, and write $\{1, 2, 3, 4\} = \{1, \iota\} \amalg \{\kappa, \lambda\}$. Let $v_n(\iota)$ be the largest integer v such that B_n is divisible by t_ι^v. From (6.2.2) and (6.1.1) we find

$$\begin{aligned} v_n(\iota) &= \max\bigl\{0, (p-1) - q \cdot [-na_\kappa]_m - q \cdot [-na_\lambda]_m\bigr\} \\ &= \max\bigl\{0, q \cdot [na_\kappa]_m + q \cdot [na_\lambda]_m - (p-1)\bigr\} \,, \end{aligned}$$

and similarly for $v_{-n}(\iota)$.
Next let $w_{\pm n}(\iota)$ be the largest integer w such that $B_n \cdot B_{-n}$ is divisible by t_ι^w. We find

$$\begin{aligned} w_{\pm n}(\iota) = \max&\bigl\{0, q \cdot [na_\kappa]_m + q \cdot [na_\lambda]_m - (p-1)\bigr\} \\ &+ \max\bigl\{0, q \cdot [-na_\kappa]_m + q \cdot [-na_\lambda]_m - (p-1)\bigr\} \,, \end{aligned}$$

which by (6.1.1) we can rewrite as

$$\begin{aligned} w_{\pm n}(\iota) &= \max\bigl\{0, q \cdot [na_\kappa]_m + q \cdot [na_\lambda]_m - (p-1)\bigr\} \\ &\quad + \max\bigl\{0, q \cdot [na_1]_m + q \cdot [na_\iota]_m - (p-1)\bigr\} \\ &= q \cdot \max\bigl\{[na_1]_m + [na_\iota]_m, [na_\kappa]_m + [na_\lambda]_m\bigr\} - (p-1) \,. \end{aligned} \tag{6.2.3}$$

(6.3) *Lemma.* — *Consider two 4-tuples* (b_1, b_2, b_3, b_4) *and* (b'_1, b'_2, b'_3, b'_4) *in* $\{1, \ldots, m-1\}^4$ *with* $\sum_{i=1}^4 b_i = 2m = \sum_{i=1}^4 b'_i$. *Suppose that for all partitions* $\{1, 2, 3, 4\} = \{1, \iota\} \amalg \{\kappa, \lambda\}$ *we have* $\{b_1 + b_\iota, b_\kappa + b_\lambda\} = \{b'_1 + b'_\iota, b'_\kappa + b'_\lambda\}$ *as sets. Then there is an even permutation* $\sigma \in A_4$ *of order* 2 *such that either* $b'_i = b_{\sigma(i)}$ *for all* i *or* $b'_i = m - b_{\sigma(i)}$ *for all* i.

Proof. Straightforward checking of all $8 = 2^3$ possible combinations (two for each partition). □

(6.4) The relation (6.2.1) implies that for any partition $\{1, 2, 3, 4\} = \{1, \iota\} \amalg \{\kappa, \lambda\}$ we have $w_{\pm n}(\iota) = w_{\pm n'}(\iota)$. Since $\sum_{i=1}^4 [na_i]_m = 2m = \sum_{i=1}^4 [n'a_i]_m$, it follows from (6.2.3) that

$$\big\{[na_1]_m + [na_\iota]_m, [na_\kappa]_m + [na_\lambda]_m\big\} = \big\{[n'a_1]_m + [n'a_\iota]_m, [n'a_\kappa]_m + [n'a_\lambda]_m\big\}$$

as sets. By the lemma it follows, possibly after replacing n by $-n$, which we may do, that there is an even permutation $\sigma \in A_4$ of order 2 such that $[n'a_i]_m = [na_{\sigma(i)}]_m$ for all i. As the pairs $\pm n$ and $\pm n'$ are distinct, $\sigma \neq 1$. Possibly after a permutation of the indices we may therefore assume that

$$\begin{aligned} [n'a_1]_m &= [na_2]_m\,, \qquad & [n'a_3]_m &= [na_4]_m\,, \\ [n'a_2]_m &= [na_1]_m\,, \qquad & [n'a_4]_m &= [na_3]_m\,. \end{aligned} \tag{6.4.1}$$

Since $\gcd(m, a_1, \ldots, a_4) = 1$ this implies that $\gcd(m, n) = \gcd(m, n')$.

(6.5) Let $r = \gcd(n, m)$. Let $m' = m/r$, and consider the triple (m', N', a') obtained from (m, N, a) by reduction modulo m'. Then we have a bijection $\mathscr{D}(m, a) \xrightarrow{\sim} \mathscr{D}(m', a')$ by $(\pm n) \mapsto (\pm \frac{n}{r})$. Hence $\#\mathscr{D}(m', a') \geqslant 2$. In particular, $N' = 4$, and (m', N', a') is not equivalent to one of the triples listed in Table 1. By our minimality assumption on (m, N, a), see 5.4, it therefore follows that $r = 1$. Hence we may replace the 4-tuple a by $n'a = (n'a_1, \ldots, n'a_4)$, which means we may set $n' = 1$ in the above. In this case, (6.4.1) tells us that $n^2 = 1$ in $(\mathbb{Z}/m\mathbb{Z})$, and the 4-tuple a has the form $a = (a_1, na_1, a_3, na_3)$ with $n \neq \pm 1$ and

$$(n+1)(a_1 + a_3) = 2m\,. \tag{6.5.1}$$

From these relations we want to deduce that there is a pair $\pm\nu \in \mathscr{D}(m, a)$ with $\gcd(m, \nu) \neq 1$, thereby obtaining a contradiction. Write $m = 2^k \cdot M$ with M odd.

First assume $n \not\equiv -1$ modulo M. For an odd prime number ℓ and an exponent $e \geqslant 1$, the congruence $n^2 \equiv 1 \bmod \ell^e$ only has $n \equiv \pm 1$ as solutions. Hence there is an odd prime divisor ℓ of m such that $n \not\equiv -1 \bmod \ell$. But then (6.5.1) gives $a_1 + a_3 \equiv 0 \bmod \ell$, and since $\gcd(m, a_1, \ldots, a_4) = 1$ we further have $a_1 \not\equiv 0 \bmod \ell$ and $a_3 \not\equiv 0 \bmod \ell$. Taking $\nu := m/\ell$ we find that $\pm\nu \in \mathscr{D}(m, a)$; contradiction.

The only remaining possibility is that $n \equiv -1$ modulo M, and therefore $n \not\equiv -1 \bmod 2^k$. In particular, $k \geqslant 2$. In this case (6.5.1) implies $a_1 + a_3 \equiv 0 \bmod 4$, in which case $\pm m/4 \in \mathscr{D}(m,a)$; contradiction. This completes the proof of Thm. 3.6 in the case $N = 4$.

7. Proof of the main result: five or more branch points

We now turn to the case $N \geqslant 5$. The idea behind the proof is the same as in the previous section, but there are some additional difficulties. In 7.2 and 7.3 we prove two technical results. Once we have these, we can again write down elements in the source of the map (5.8.1). Similar to what we did in Section 6, this gives us polynomial identities (7.4.1), and with some elementary combinatorial arguments we can then conclude the proof.

(7.1) *Assumptions.* — We retain the assumptions made in 5.4. In addition we now assume $N \geqslant 5$. Again we assume (m, N, a) is minimal. Because we have already proven Thm. 3.6 for $N = 4$, it is again true that if m' is a proper divisor of m and (m', N', a') is obtained from (m, N, a) by reduction modulo m', either $N' \leqslant 3$ or (m', N', a') is equivalent to one of the twenty triples listed in Table 1.

(7.2) *Lemma.* — *With assumptions as in* 7.1, *there exists an index $n \in (\mathbb{Z}/m\mathbb{Z})^*$ such that $\{d_n, d_{-n}\} \neq \{0, N-2\}$.*

With the terminology introduced in 4.3, the lemma says that the new part of the local system $\mathbb{V}$ (as in Section 4) is not isotrivial.

Proof. We assume $\{d_n, d_{-n}\} = \{0, N-2\}$ for all $n \in (\mathbb{Z}/m\mathbb{Z})^*$, and we seek to derive a contradiction. It will be convenient to consider the function $\delta_a\colon \mathbb{Z}/m\mathbb{Z} \to \mathbb{Z}_{\geqslant 0}$ given by $\delta_a(n) = \sum_{i=1}^N \left\langle \frac{-na_i}{m} \right\rangle$. Note that for $n \neq 0$ the d_n defined in (3.2.2) equals $-1 + \delta_a(n)$. For $n \in (\mathbb{Z}/m\mathbb{Z})^*$ we have $\delta_a(n) \geqslant 1$ and $\delta_a(n) + \delta_a(-n) = N$. Our assumption is equivalent to the condition that

$$\{\delta_a(n), \delta_a(-n)\} = \{1, N-1\} \quad \text{for all } n \in (\mathbb{Z}/m\mathbb{Z})^*. \tag{7.2.1}$$

Possibly after replacing $a = (a_1, \ldots, a_N)$ by $-a$, we may assume $\delta_a(1) = 1$, which means that

$$[a_1]_m + \cdots + [a_N]_m = m\,. \tag{7.2.2}$$

We divide the proof into a couple of steps.

Step 1. Our first goal is to show that $m > 60$. For a given m, (7.2.2) leaves only finitely many possible triples (m, N, a), up to equivalence. With the help of a small computer program we check that for $m \leqslant 60$ the only two possibilities with $N \geqslant 5$ and $\{\delta_a(n), \delta_a(-n)\} = \{1, N-1\}$ for all $n \in (\mathbb{Z}/m\mathbb{Z})^*$ are given (up to equivalence) by

$$m = 6\,, \quad N = 5\,, \quad a = (1,1,1,1,2)\,; \tag{7.2.3}$$

(7.2.4) $$m = 6\,, \quad N = 6\,, \quad a = (1,1,1,1,1,1)\,.$$

So it remains to show that for these triples, $Z(m,N,a)$ is not special.
In case (7.2.3), we have $g = 7$ and the family of Jacobians $J \to T$ decomposes, up to isogeny, as a product of three factors: $J \sim Y_1 \times Y_2 \times Y_3$, with
— Y_1 a pull-back of the Legendre family of elliptic curves, which is Example 1 in Table 1; this is the old factor corresponding to the divisor 2 of m,
— Y_2 a pull-back of Example 6; this is the old factor corresponding to the divisor 3 of m,
— Y_3 the new part.

(The new part Y_3 is in fact an isotrivial family of 3-dimensional abelian varieties of CM type, but we will not need this.) Let $b \in T(\mathbb{C})$ be a Hodge-generic point. The fibre $Y_{1,b}$ is an elliptic curve with endomorphism ring $\mathbb{Z}$; its Hodge group is isomorphic with SL_2. The fibre $Y_{2,b}$ is an abelian threefold that is easily seen to be simple. (E.g., use the fact that Example 6 is special, together with [23], Thm. 5.) By [16], Prop. 3.8 the Hodge group of $Y_{1,b} \times Y_{2,b}$ is the product of the two Hodge groups. Hence the smallest special subvariety $S \subset \mathscr{A}_7$ that contains $Z(m,N,a)$ has dimension at least $1+2=3$ (see 1.5), and since $N-3 = 2 < 3$ this means that $Z(m,N,a)$ is not special.
In case (7.2.4), we have $g = 10$ and the family of Jacobians $J \to T$ decomposes, up to isogeny, as a product of three factors: $J \sim Y_1 \times Y_2 \times Y_3$, with
— Y_1 a pull-back of Example 2; this is the old factor corresponding to the divisor 2 of m,
— Y_2 a pull-back of Example 10; this is the old factor corresponding to the divisor 3 of m,
— Y_3 the new part.

(In this case the new part Y_3 is an isotrivial family of 4-dimensional abelian varieties of CM type; again we will not need this.) For a Hodge-generic point $b \in T(\mathbb{C})$ the fibre $Y_{1,b}$ is an abelian surface with endomorphism ring $\mathbb{Z}$; its Hodge group $H_1 = \mathrm{Hdg}(Y_{1,b})$ is isomorphic with Sp_4. The fibre $Y_{2,b}$ is an abelian fourfold. By Thm. 1.1 of [26] we have $\mathrm{End}(Y_{2,b}) = \mathbb{Z}[\zeta_3]$, and the tangent multiplicities for the factor Y_2 (=Example 10) are given by $d_{(1 \bmod 3)} = 3$ and $d_{(2 \bmod 3)} = 1$. By [15], 7.4, it follows that for the generic Hodge group $H_2 = \mathrm{Hdg}(Y_{2,b})$ we have $H_{2,\mathbb{R}} \cong \mathrm{U}(1,3)$. If $H = \mathrm{Hdg}(J_b)$ is the generic Hodge group in our family of Jacobians, H projects surjectively to H_1 and H_2. It follows that among the simple factors of $H_{\mathbb{R}}^{\mathrm{ad}}$ both a factor PSp_4 and a factor $\mathrm{PSU}(1,3)$ occur; this implies that the smallest special subvariety $S \subset \mathscr{A}_7$ that contains $Z(m,N,a)$ has dimension at least $3+3=6$ (again see 1.5), and since $N-3 = 3 < 6$ this means that $Z(m,N,a)$ is not special.

Step 2. The function δ_a has the property that $\delta_a(n_1+n_2) \leqslant \delta_a(n_1) + \delta_a(n_2)$. In particular, if n_1, n_2 and n_1+n_2 are all in $(\mathbb{Z}/m\mathbb{Z})^*$ then by (7.2.1) we have the implication

(7.2.5) $$\delta_a(n_1) = \delta_a(n_2) = 1 \quad \Rightarrow \quad \delta_a(n_1+n_2) = 1\,.$$

Step 3. Next we show that m is not divisible by 2, 3 or 5. Let $p \in \{2,3,5\}$, and suppose m is divisible by p. Let $m' = m/p$ and let (m', N', a') be obtained from (m, N, a) by reduction modulo m'. The new triple cannot be one of the examples listed in Table 1, for this would imply (by inspection of the table) that $m = p \cdot m' \leqslant 5 \cdot 12 = 60$, which we have excluded. Hence our minimality assumption on the triple (m, N, a) implies that $N' \leqslant 3$.
Since $N \geqslant 5$, there are at least two indices i such that $a_i \equiv 0$ modulo m'. For $p = 2$ this contradicts (7.2.2). Hence $2 \in (\mathbb{Z}/m\mathbb{Z})^*$ and by repeated application of (7.2.5), starting from $\delta_a(1) = 1$, we find that $\delta_a(2^k) = 1$ for all k.
For $p = 3$ the only possibility left, in view of (7.2.2), is that there are precisely two indices i with $[a_i]_m = m/3$ and that $[a_i]_m < m/3$ for all remaining indices. This contradicts the fact that $\delta_a(2) = 1$. Hence 3 does not divide m.
Finally take $p = 5$. The fact that $\delta_a(2) = 1$ implies that there is a unique index i with $[a_i]_m > m/2$ and that $[a_i]_m < m/2$ for all remaining indices. Since $N \geqslant 5$ and $N' \leqslant 3$ this leaves (possibly after a permutation of the indices) two possibilities: either

$$[a_1]_m = 3m/5\,, \quad [a_2]_m = m/5\,, \quad [a_i]_m < m/5 \quad \text{for all } i > 2,$$

or

$$m/2 < [a_1]_m < 3m/5\,, \quad [a_2]_m = [a_3]_m = m/5\,, \quad [a_i]_m < m/5 \quad \text{for all } i > 3.$$

In both cases we get a contradiction with the fact that $\delta_a(4) = 1$.

Step 4. We now show that m has at most four distinct prime divisors. To see this, let p be any prime divisor of m, let $m' = m/p$ and let (m', N', a') be obtained from (m, N, a) by reduction modulo m'. If the new triple is one of the examples listed in Table 1, it can only be Example 17, for otherwise inspection of the table gives that m' (and hence m) is divisible by 2, 3, or 5, which we have excluded. Example 17 has $N' = 4$ branch points, so this fact, together with our minimality assumption on the triple (m, N, a), implies that $N' \leqslant 4$.
The previous argument shows that for any prime divisor p of m, there are at most 4 indices i such that a_i is not divisible by m/p. On the other hand, $a_i \not\equiv 0 \bmod m$, so for a given index i there can be at most one prime divisor p of m such that a_i is divisible by m/p. As $N \geqslant 5$ it follows that m has at most four distinct prime divisors.

Step 5; conclusion of the proof. Combining the conclusion of Step 3 with (7.2.5), we find that for all $\rho \in \{1,2,3,4,5\}$ we have $(\rho \bmod m) \in (\mathbb{Z}/m\mathbb{Z})^*$ and $\delta_a(\rho \bmod m) = 1$.
Let ν be an integer such that $\gcd(m, \nu) = 1$ and $\delta_a(\nu \bmod m) = 1$. Let ρ be the smallest positive integer such that $\gcd(m, \nu + \rho) = 1$. The fact that m has at most four distinct prime divisors, all greater than 5, implies that $\rho \leqslant 5$. But then $\gcd(\rho, m) = 1$ and from (7.2.5) we get that $\delta_a(\nu + \rho \bmod m) = 1$. Repeating this, we find that $\delta_a(n) = 1$ for all $n \in (\mathbb{Z}/m\mathbb{Z})^*$, which contradicts the fact that $\delta_a(n) + \delta_a(-n) = N > 3$. This completes the proof of the lemma. □

(7.3) Our next goal is to show there exist two distinct pairs $\pm n$ and $\pm n'$ in $I(m)$ with

$$d_{-n} = d_{-n'} = 1\,, \quad \text{and} \quad d_n = d_{n'} = N-3\,. \tag{7.3.1}$$

(In particular, $n \not\equiv 0$ and $n' \not\equiv 0$.) For this we work over $\mathbb{C}$ and we consider the generic Mumford-Tate group M of the family C/T. As in 1.5, let $M_{\mathbb{R}}^{\mathrm{ad}} = Q_1 \times \cdots \times Q_r$ be the decomposition of $M_{\mathbb{R}}^{\mathrm{ad}}$ as a product of simple factors. The assumption that $Z(m,N,a)$ is special means that $N-3 = \sum_{i=1}^r d(Q_i)$, with notation as in 1.5. Further, this assumption implies that the connected algebraic monodromy group Mon^0 of the family is a normal subgroup of M; in particular, $\mathrm{Mon}_{\mathbb{R}}^{0,\mathrm{ad}} = \prod_{i\in K} Q_i$ for some subset $K \subset \{1,\dots,r\}$.
By Lemma 7.2 there exists an index n in $(\mathbb{Z}/m\mathbb{Z})^*$ with $\{d_n, d_{-n}\} \neq \{0, N-2\}$. By Prop. 4.7 it follows that one of the simple factors Q_i, say Q_1, is a $\mathrm{PSU}(d_n, d_{-n})$, which gives $d(Q_1) = d_n d_{-n}$. Because $n \in (\mathbb{Z}/m\mathbb{Z})^*$ we have $d_n + d_{-n} = N-2$; hence $d_n d_{-n} \geqslant N-3$ with equality of and only if $\{d_n, d_{-n}\} = \{1, N-3\}$. Possibly after replacing n by $-n$ we therefore have $d_n = N-3$ and $d_{-n} = 1$. Further, the relation $N-3 = \sum_{i=1}^r d(Q_i)$ implies that all other simple factors $Q_2,\dots,Q_r$ are anisotropic (i.e., compact).
Our assumptions imply that there is another index pair $\pm n' \in I(m)$ with $d_{n'} \neq 0$ and $d_{-n'} \neq 0$, for if this is not the case then (m,N,a) satisfies (4.8.1), which implies it is one of the examples of Table 1. If $m = 2m'$ is even and $n' = m'$ then by Prop. 4.7 one of the factors Q_i is a PSp_{2h} with $h = d_{n'} > 0$. As $N-3 \geqslant 2$, this factor cannot be the factor $Q_1 = \mathrm{PSU}(1, N-3)$, and since PSp_{2h} is not anisotropic we arrive at a contradiction. So $n' \neq -n'$, and, again by Prop. 4.7, one of the Q_i is a non-compact unitary factor $\mathrm{PSU}(d_{n'}, d_{-n'})$. This factor must be the factor Q_1; hence $\{d_{n'}, d_{-n'}\} = \{1, N-3\}$, which gives what we want.

(7.4) Consider two distinct pairs $\pm n$ and $\pm n'$ in $I(m)$ for which (7.3.1) holds. Let $\Gamma \in \mathrm{GL}_{N-3}(\mathscr{O}_U)$ be the matrix of $\gamma_{(n)}\colon F_U^*\mathbb{E}_{U,(n)} \to \mathbb{E}_{U,(n)}$ with regard to the frames given by the forms $\omega_{n,\sigma}$. It is the inverse of the matrix $A = A_n$ of Lemma 5.9. Similarly, let Γ' be the matrix of $\gamma_{(n')}$, and let $A' = A_{n'}$ be its inverse. Further, let c and c' be the sections of $\mathscr{O}_U^*$ (the inverses of the 1×1 matrices A_{-n} and $A_{-n'}$ of Lemma 5.9) such that $\gamma(\omega_{-n,0}\otimes 1) = c\cdot\omega_{-n,0}$ and $\gamma(\omega_{-n',0}\otimes 1) = c\cdot\omega_{-n',0}$.
For $\sigma \in \{0,1,\dots,N-4\}$, let $\eta_\sigma \in \Gamma(U, \mathscr{K}_{(0)})$ be given by

$$\eta_\sigma := \omega_{-n,0}\otimes\omega_{n,\sigma} - \omega_{-n',0}\otimes\omega_{n',\sigma}\,.$$

As $\omega_{-n,0}\cdot\omega_{n,\rho} = \omega_{-n',0}\cdot\omega_{n',\rho}$ as sections of $f_*(\omega^{\otimes 2})$, the image of η_σ under $\mathrm{Sym}^2(\gamma)$ equals

$$\sum_{\rho=0}^{N-4} \left(c\cdot\Gamma_{\rho,\sigma} - c'\cdot\Gamma'_{\rho,\sigma}\right)\cdot\left(\omega_{-n,0}\cdot\omega_{n,\rho}\right).$$

Because the sections $\omega_{-n,0}\cdot\omega_{n,\rho}$ for $\rho \in \{0,\dots,N-4\}$ are linearly independent, it follows from Prop. 5.8 that $c\cdot\Gamma_{\rho,\sigma} - c'\cdot\Gamma'_{\rho,\sigma}$ for all σ, $\rho \in \{0,1,\dots,N-4\}$, which can be rewritten as

$$c^{-1}\cdot A_{\rho,\sigma} = c^{\prime,-1}\cdot A'_{\rho,\sigma}\,. \tag{7.4.1}$$

Choose two distinct indices κ, λ in $\{1,2,\dots,N\}$, and write $\{1,\dots,N\} = \{\kappa,\lambda\} \amalg I$. For $\nu \in \{0,1\}$, define $v_n(\nu)$ to be the largest integer v such that $A_{\nu,\nu}|_{t_\kappa=0}$ is divisible by t_λ^v. Similarly, let v_{-n} be the largest integer v such that $c^{-1}|_{t_\kappa=0}$ is divisible by t_λ^v. Using the explicit formulas for c^{-1} and the matrix A from Lemma 5.9, we find

$$\begin{aligned} v_{-n} &= \max\Big\{0,(p-1)-q\cdot\sum_{i\in I}[na_i]_m\Big\}\,,\\ v_n(0) &= \max\Big\{0,(N-3)(p-1)-q\cdot\sum_{i\in I}[-na_i]_m\Big\}\,,\\ v_n(1) &= 0\,. \end{aligned}$$

(Recall that $q=(p-1)/m$.)
Next we define $w_n(\nu) = v_{-n} + v_n(\nu)$ to be the largest integer w such that $\big(c^{-1}\cdot A_{\nu,\nu}\big)|_{t_\kappa=0}$ is divisible by t_λ^w. Similar to (6.1.1), it follows from the fact that $d_{-n}=1$ and $d_n = N-3$ that $[-na_i]_m = m-[na_i]_m$ for all i and $\sum_{i=1}^N [na_i]_m = 2m$. Using these relations we obtain

$$\begin{aligned} w(0) &= \max\Big\{(p-1)-q\cdot\sum_{i\notin I}[na_i]_m, (p-1)-q\cdot\sum_{i\in I}[na_i]_m\Big\}\\ &= \Big|(p-1)-q\cdot\sum_{i\notin I}[na_i]_m\Big| = q\cdot\big|m-[na_\kappa]_m-[na_\lambda]_m\big|\,,\\ w(1) &= \max\Big\{0,(p-1)-q\cdot\sum_{i\in I}[na_i]_m\Big\}\\ &= \max\Big\{0,(p-1)-q\cdot\sum_{i\notin I}[na_i]_m\Big\} = q\cdot\max\big\{0,[na_\kappa]_m+[na_\lambda]_m-m\big\}\,. \end{aligned}$$

We can do the same calculations for the pair $\pm n'$; let us call $w'(0)$ and $w'(1)$ the resulting values. From (7.4.1) we get the relations $w(0) = w'(0)$ and $w(1) = w'(1)$. It follows that for all choices of κ and λ we have $[na_\kappa]_m + [na_\lambda]_m = [n'a_\kappa]_m + [n'a_\lambda]_m$. This readily implies that $[na_i]_m = [n'a_i]_m$ for all $i \in \{1,\dots,N\}$. As $\gcd(m,a_1,\dots,a_N)=1$ it follows that $n=n'$, which contradicts our assumption that the pairs $\pm n$ and $\pm n'$ are distinct. This completes the proof of Theorem 3.6. □

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Duality and Integrability on Contact Fano Manifolds

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Abstract. We address the problem of classification of contact Fano manifolds. It is conjectured that every such manifold is necessarily homogeneous. We prove that the Killing form, the Lie algebra grading and parts of the Lie bracket can be read from geometry of an arbitrary contact manifold. Minimal rational curves on contact manifolds (or contact lines) and their chains are the essential ingredients for our constructions.

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1 Introduction

In this article we are interested in the classification of contact Fano manifolds. We review the relevant definitions in §2. So far the only known examples of contact Fano manifolds are obtained as follows. For a simple Lie group G consider its adjoint action on $\mathbb{P}(\mathfrak{g})$, where $\mathfrak{g}$ is the Lie algebra of G. This action has a unique closed orbit X and this X has a natural contact structure. In this situation X is called a *projectivised minimal nilpotent orbit*, or the *adjoint variety* of G. By the duality determined by the Killing form, equivalently we can consider the coadjoint action of G on $\mathbb{P}(\mathfrak{g}^*)$ and X is isomorphic to the unique closed orbit in $\mathbb{P}(\mathfrak{g}^*)$.

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Conjecture 1.1 (LeBrun, Salamon). *If X is a Fano complex contact manifold, then X is the adjoint variety of a simple Lie group G.*

This problem originated with a problem in Riemannian geometry. In [Ber55] a list of all possible holonomy groups of simply connected Riemannian manifolds is given. The existence problem for all the cases has been solved locally. Also compact non-homogeneous examples with most of the possible holonomy groups were constructed with the unique exception of the quaternion-Kähler manifolds. It is conjectured that the compact quaternion-Kähler manifolds must be homogeneous (see [LeB95] and references therein).

Conjecture 1.2 (LeBrun, Salamon). *Let M be a compact quaternion-Kähler manifold. Then M is a homogeneous symmetric space (more precisely, it is one of the Wolf spaces — see [Wol65]).*

The relation between the conjectures is given by the construction of a twistor space. The S^2-bundle of complex structures on tangent spaces to a quaternion-Kähler manifold M is called the twistor space of M. If M is compact, it has positive scalar curvature, and then the twistor space X has a natural complex structure and is a contact Fano manifold with a Kähler-Einstein metric. In particular, the twistor space of a Wolf space is an adjoint variety. Hence Conjecture 1.1 implies Conjecture 1.2. Conversely, if X is a contact Fano manifold with Kähler-Einstein metric, then it is a twistor space of a quaternion-Kähler manifold — see [LeB95].

In order to study the non-homogeneous contact manifolds (potentially non-existent) it is natural to assume $\operatorname{Pic} X \simeq \mathbb{Z}$ and further that X is not isomorphic to a projective space. This only exludes the adjoint varieties of types A and C (see §2 for more details).

With this assumption, we take a closer look at three pieces of the homogeneous structure on adjoint varieties: the Killing form B on $\mathfrak{g}$, the Lie algebra grading $\mathfrak{g} = \mathfrak{g}_{-2} \oplus \mathfrak{g}_{-1} \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_2$ (see [LM02, §6.1] and references therein) and a part of the Lie bracket on $\mathfrak{g}$. Understanding the underlying geometry allows us to define the appropriate generalisations of these notions on arbitrary contact Fano manifolds.

An essential building block for our constructions is the notion of a *contact line* (or simply *line*) on X. These contact lines were studied by Kebekus [Keb01], [Keb05] and Wiśniewski [Wiś00]. Also they are an instance of minimal rational curves, which are studied extensively. The geometry of contact lines was the original motivation to study Legendrian subvarieties in projective space (see [Bucz09] for an overview and many details). We briefly review the subject of lines on contact Fano manifolds in §3.1.

The key ingedient is the construction of a family of divisors D_x parametrised by points $x \in X$ (see §3.3). These divisors are swept by pairs of intersecting contact lines, one of which passes through x. In other words, set theoretically D_x is the set of points of X, which can be joined with x using at most 2 intersecting contact lines. The idea to study these loci comes from Wiśniewski [Wiś00] where he observed, that (under an additional minor assumption) these loci contain some non-trivial divisorial components and he studied the intersection numbers of certain curves on X with the divisorial components. Here we prove all the components of D_x are divisorial and draw conclusions from that observation going into a different direction than those of [Wiś00].

Theorem 1.3. *Let X be a contact Fano manifold with $\operatorname{Pic} X \simeq \mathbb{Z}$ and assume X is not isomorphic to a projective space. Then the locus $D_x \subset X$ swept by the pairs of intersecting contact lines, one of which passes through $x \in X$ is of pure codimension 1 and thus D_x determines a divisor on X. Let $\langle D \rangle \subset H^0(\mathcal{O}(D_x))$ be the linear system spanned by these divisors. Let $\phi\colon X \to \mathbb{P}\langle D \rangle^*$ be the map determined by the linear system $\langle D \rangle$ and let $\psi\colon X \to \mathbb{P}\langle D \rangle$ be the map $x \mapsto D_x$. Then:*

(i) both ϕ and ψ are regular maps.

(ii) there exists a unique up to scalar non-degenerate bilinear form B on $\langle D \rangle$, which determines an isomorphism $\mathbb{P}\langle D \rangle^* \simeq \mathbb{P}\langle D \rangle$ making the following diagram commutative:

$$\begin{array}{ccc} & \overset{\phi}{\nearrow} & \mathbb{P}\langle D \rangle^* \\ X & & \big\downarrow \simeq \\ & \underset{\psi}{\searrow} & \mathbb{P}\langle D \rangle. \end{array}$$

(iii) The bilinear form B is either symmetric or skew-symmetric.

(iv) If $X \subset \mathbb{P}(\mathfrak{g}^*)$ is the adjoint variety of simple Lie group G, then $\langle D \rangle = \mathfrak{g}$ and B is the Killing form on $\mathfrak{g}$.

With the notation of the theorem, after fixing a pair of general points $x, w \in X$ there are certain natural linear subspaces of $\langle D \rangle$, which we denote $\langle D \rangle_{-2}$, $\langle D \rangle_{-1}$, $\langle D \rangle_0$, $\langle D \rangle_1$ and $\langle D \rangle_2$ (see §5 for details).

Theorem 1.4. *If $X \subset \mathbb{P}(\mathfrak{g}^*)$ is the adjoint variety of a simple Lie group G with $\operatorname{Pic} X \simeq Z$ and X not isomorphic to a projective space, then there exists a choice of a maximal torus of G and a choice of order of roots of $\mathfrak{g}$, such that $\langle D \rangle_i = \mathfrak{g}_i$ for every $i \in \{-2, -1, 0, 1, 2\}$, where $\mathfrak{g} = \mathfrak{g}_{-2} \oplus \mathfrak{g}_{-1} \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_2$ is the Lie algebra grading of $\mathfrak{g}$.*

Finally, if X is the adjoint variety of G, then there is a rational map

$$[\cdot,\cdot]\colon X \times X \dashrightarrow \mathbb{P}(\mathfrak{g}),$$

which is the Lie bracket on $\mathfrak{g}$ (up to projectivisation). Also there is a divisor $D \subset X \times X$, such that for general $(x, z) \in D$ the Lie bracket $[x, z]$ is in X. We recover this bracket restricted to D for general contact manifolds:

Theorem 1.5. *For X and D_x and in Theorem 1.3, let $D \subset X \times X$ be the divisor consisting of pairs $(x, z) \in X \times X$, such that $z \in D_x$. There exists a rational map $[\cdot,\cdot]^D : D \dashrightarrow X$, such that $[x, z]^D = y$, where y is an intersection point of a pair of contact lines that join x and z. In particular, this intersection point y and the pair of lines are unique for general pair $(x, z) \in D$. Moreover, if X is the adjoint variety of a simple Lie group G, then $[\cdot,\cdot]^D$ is the restricion of the Lie bracket.*

In §2 we introduce and motivate our assumptions and notation.
In §3 we review the notion of contact lines and their properties. We continue by studying certain types of loci swept by those lines and calculate their dimensions. In particular we prove there Theorem 3.6, which is a part of results summarised in Theorem 1.3. We also study the tangent bundle to D_x as a subspace of TX.
In §4 we study the duality of maps ϕ and ψ introduced in Theorem 1.3 together with the consequences of this duality. This section is culminated with the proof of Theorem 1.3.
In §5 we generalise the Lie algebra grading to arbitrary contact manifolds and prove Theorem 1.4.
In §6 we prove that certain lines are integrable with respect to a special distribution on D_x and we apply this to prove Theorem 1.5.

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2 Preliminaries

Throughout the paper all our projectivisations $\mathbb{P}$ are naive. This means, if V is a vector space, then $\mathbb{P}V = (V \setminus 0)/\mathbb{C}^*$, and similarly for vector bundles.
A complex manifold X of dimension $2n+1$ is *contact* if there exists a vector subbundle $F \subset TX$ of rank $2n$ fitting into an exact sequence:

$$0 \to F \to TX \xrightarrow{\theta} L \to 0$$

such that the derivative $\mathrm{d}\theta \in H^0(\bigwedge^2 F^* \otimes L)$ of the twisted form $\theta \in H^0(T^*X \otimes L)$ is nowhere degenerate. In particular, $\mathrm{d}\theta_x$ is a symplectic form on the fibre of contact distribution F_x. See [Bucz09, §E.3 and Chapter C] and references therein for an overview of the subject.
A projective manifold X is Fano, if its anticanonical divisor $K_X{}^* = \bigwedge^{\dim X} TX$ is ample.

If X is a projective contact manifold, then by Theorem of Kebekus, Peternell, Sommese and Wiśniewski [KPSW00] combined with a result by Demailly [Dem02], X is either a projectivisation of a cotangent bundle to a smooth projective manifold or X is a contact Fano manifold, with $\operatorname{Pic} X \simeq \mathbb{Z}$. In the second case, since $K_X \simeq (L^*)^{\otimes(n+1)}$, by [KO73], either $X \simeq \mathbb{P}^{2n+1}$ or $\operatorname{Pic} X = \mathbb{Z} \cdot [L]$. Here we are interested in the case $X \not\simeq \mathbb{P}^{2n+1}$. Thus our assumption spelled out below only exclude some well understood cases (the projectivised cotangent bundles and the projective space) and they agree with the assumptions of Theorems 1.3, 1.4 and 1.5.

Notation 2.1. Throughout the paper X denotes a contact Fano manifold with $\operatorname{Pic} X$ generated by the class of L, where $L = TX/F$ and $F \subset TX$ is the contact distribution on X. We also assume $\dim X = 2n + 1$.

From Theorem of Ye [Ye94] it follows that $n \geq 2$.
We will also consider the homogeneous examples of contact manifolds (i.e. the adjoint varieties). Thus we fix notation for the Lie group and its Lie algebra.

Notation 2.2. Throughout the paper G denotes a simple complex Lie group, not of types A or C (i.e. not isomorphic to SL_n nor Sp_{2n} nor their discrete quotients). Further $\mathfrak{g}$ is the Lie algebra of G. Thus $\mathfrak{g}$ is one of $\mathfrak{so}_n$ (types B and D), or one of the exceptional Lie algebras $\mathfrak{g}_2$, $\mathfrak{f}_4$, $\mathfrak{e}_6$, $\mathfrak{e}_7$ or $\mathfrak{e}_8$.

The contact structure on $\mathbb{P}^{2n-1} = \mathbb{P}(\mathbb{C}^{2n})$ is determined by a symplectic form ω on $\mathbb{C}^{2n}$. The precise relation between the contact and symplectic structures is decribed for instance in [Bucz09, §E.1] (see also [LeB95, Ex. 2.1]). In particular, for all $x \in X$, the projectivisation of a fibre of the contact distribution $\mathbb{P}F_x$ comes with a natural contact structure.
Let M be a projective contact manifold (in our case $M = X$ with X as in Notation 2.1 or $M = \mathbb{P}^{2n-1}$). A subvariety $Z \subset M$ is *Legendrian*, if for all smooth points $z \in Z$ the tangent space $T_z Z$ is contained in the contact distribution of M and Z is of pure dimension $\frac{1}{2}(\dim M - 1)$.
Recall from [Har95, Lecture 20] or [Mum99, III.§3,§4] the notion of *tangent cone*. For a subvariety $Z \subset X$, and a point $x \in Z$ let $\tau_x Z \subset T_x X$ be the tangent cone of Z at x. In this article we will only need the following elementary properties of the tangent cone:

- $\tau_x Z$ is an affine cone (i.e. it is invariant under the standard action of $\mathbb{C}^*$ on $T_x X$).
- $\dim_x Z = \dim \tau_x Z$ and thus if Z is irreducible, then $\dim Z = \dim \tau_x Z$.
- If $x \in Z_1 \subset Z_2 \subset X$, then $\tau_x Z_1 \subset \tau_x Z_2$.
- If Z is smooth at x, then $\tau_x Z = T_x Z$.

Since $\tau_x Z$ is a cone, let $\mathbb{P}\tau_x Z \subset \mathbb{P}T_x X$ be the corresponding projective variety.

3 Loci swept out by lines

A rational curve $l \subset X$ is a *contact line* (or simply a *line*) if $\deg L|_l = 1$.
Let $RatCurves^n(X)$ be the normalised scheme parametrising rational curves on X, as in [Kol96, II.2.11]. Let $Lines(X) \subset RatCurves^n(X)$ be the subscheme parametrising lines. Then every component of $Lines(X)$ is a minimal component of X in the sense of [HM04]. We fix $\mathcal{H} \neq \emptyset$ a union of some irreducible components of $Lines(X)$.
By a slight abuse of notation, from now on we say l is a *(contact) line* if and only if $l \in \mathcal{H}$. For simplicity, the reader may choose to restrict his attention to one of the extreme cases: either to the case $\mathcal{H} = Lines(X)$ (and thus be consistent with [Wiś00] and the first sentence of this section) or to the case where $\mathcal{H}$ is one of the irreducible components of $Lines(X)$ (and thus be consistent with [Keb01, Keb05]). In general it is expected that $Lines(X)$ (with X as in Notation 2.1) is irreducible and all the cases are the same.

3.1 Legendrian varieties swept by lines

We denote by $C_x \subset X$ the locus of contact lines through $x \in X$. Let $\mathscr{C}_x := \mathbb{P}\tau_x C_x \subset \mathbb{P}(TX)$. Note that with our assumptions both C_x and $\mathscr{C}_x$ are closed subsets of X or $\mathbb{P}(T_x X)$ respectively.
The following theorem briefly summarises results of [Keb05] and earlier:

Theorem 3.1. *With X as in Notation 2.1 let $x \in X$ be any point. Then:*

(i) There exist lines through x, in particular C_x and $\mathscr{C}_x$ are non-empty.

(ii) C_x is Legendrian in X and $\mathscr{C}_x \subset \mathbb{P}(F_x)$ and $\mathscr{C}_x$ is Legendrian in $\mathbb{P}(F_x)$.

(iii) If in addition x is a general point of X, then $\mathscr{C}_x$ is smooth and each irreducible component of $\mathscr{C}_x$ is linearly non-degenerate in $\mathbb{P}(F_x)$. Further C_x is isomorphic to the projective cone over $\mathscr{C}_x \subset \mathbb{P}(F_x)$, i.e. $C_x \simeq \tilde{\mathscr{C}}_x \subset \mathbb{P}(F_x \oplus \mathbb{C})$, in such a way that lines through x are mapped bijectively onto the generators of the cone and restriction of L to C_x via this isomorphism is identified with the restriction of $\mathcal{O}_{\mathbb{P}(F_x \oplus \mathbb{C})}(1)$ to $\tilde{\mathscr{C}}_x$. In particular all lines through x are smooth and two different lines intersecting at x will not intersect anywhere else, nor they will share a tangent direction.

Proof. Part (i) is proved in [Keb01, §2.3].
The proof of (ii) is essentially contained in [KPSW00, Prop. 2.9]. Explicit statements are in [Keb01, Prop. 4.1] for C_x and in [Wiś00, Lemma 5] for $\mathscr{C}_x$. Also [HM99] may claim the authorship of this observation, since the proof in the homogeneous case is no different than in the general case.
Assume $x \in X$ is a general point. The statements of (iii) are basically [Keb05, Thm 1.1], which however assumes (in the statement) that $\mathcal{H}$ is irreducible. This is never used in the proof, with the exception of the argument for the irreducibility of C_x — see however Remark 3.2. Thus $\mathscr{C}_x$ is smooth and C_x is

isomorphic to the cone over $\mathscr{C}_x$ as claimed. Each irreducible component $\mathscr{C}_x$ is non-degenerate in $\mathbb{P}F_x$ by [Keb01, Thm 4.4] — again the statement is only for $\mathscr{C}_x$, not for its components, however the proof stays correct in this more general setup. In particular, [Keb01, Lemma 4.3] implies that C_x polarised by $L|_{C_x}$ is not isomorphic with a linear subspace with polarised by $\mathcal{O}(1)$. Thus the other results of this theorem give alternate (but more complicated) proof of that generalised non-degeneracy.

□

Remark 3.2. Note that (assuming $\mathcal{H}$ is irreducible) Kebekus [Keb05] also stated that C_x and $\mathscr{C}_x$ are irreducible for general x. However it was observed by Kebekus himself together with the author that there is a gap in the proof. This gap is on page 234 in Step 2 of proof of Proposition 3.2 where Kebekus claims to construct "a well defined family of cycles" parametrised by a divisor D^0. This is not necessarily a well defined family of cycles: Condition (3.10.4) in [Kol96, §I.3.10] is not necessarily satisfied if D^0 is not normal and there seem to be no reason to expect that D^0 is normal. As a consequence the map $\Phi\colon D^0 \to \mathrm{Chow}(X)$ is not necessarily regular at non-normal points of D^0 and it might contract some curves.

Let us define:

$$C^2 \subset X \times X$$
$$C^2 := \{(x,y) \mid y \in C_x\},$$

i.e. this is the locus of those pairs (x,y), which are both on the same contact line. Again this locus is a closed subset of $X \times X$.
Analogously, define:

$$C^3 := C^2 \times_X C^2$$

so that:

$$C^3 \subset X \times X \times X$$
$$C^3 := \{(x,y,z) \mid y \in C_x, z \in C_y\}.$$

Finally, for $x \in X$ we also define C^2_x:

$$C^2_x \subset X \times X \simeq \{x\} \times X \times X$$
$$C^2_x := \{(y,z) \mid y \in C_x, z \in C_y\},$$

with the scheme structure of the fibre of C^3 under the projection on the first coordinate. Since for all $x \in X$ all irreducible components of C_x are of dimension n (see Theorem 3.1) we conclude:

Proposition 3.3. *All C^2, C^2_x, C^3 are projective subschemes, they are all of pure dimension, and their dimensions are:*

- $\dim C^2 = 3n + 1$.

- $\dim C_x^2 = 2n$.
- $\dim C^3 = 4n + 1$.

□

3.2 Joins and secants of Legendrian subvarieties

For subvarieties $Y_1, Y_2 \subset \mathbb{P}^N$ recall that their *join* $Y_1 * Y_2$ is the closure of the locus of lines between points $y_1 \in Y_1$ and $y_2 \in Y_2$. Note that the expected dimension of $Y_1 * Y_2$ is $\dim Y_1 + \dim Y_2 + 1$. We are only concerned with two special cases: either Y_1 and Y_2 are disjoint or $Y_1 = Y_2$.

Lemma 3.4. *If $Y_1, Y_2 \subset \mathbb{P}^N$ are two disjoint subvarieties of dimensions $k-1$ and $N-k$ respectively, then their join $Y_1 * Y_2$ fills out the ambient space, i.e. this join is of expected dimension.*

Proof. Let $p \in \mathbb{P}^N$ be a general point and consider the projection $\pi : \mathbb{P}^N \dashrightarrow \mathbb{P}^{N-1}$ away from p. Let $Z_i = \pi(Y_i)$ for $i = 1, 2$. Since p is general, $\dim Z_i = \dim Y_i$ and thus $Z_1 \cap Z_2$ is non-empty. Let $q \in Z_1 \cap Z_2$ be any point. The preimage $\pi^{-1}(q)$ is a line in $\mathbb{P}^N$ intersecting both Y_1 and Y_2 and passing through p.

□

Recall, that the special case of join is when $Y = Y_1 = Y_2$ and $\sigma_2(Y) := Y * Y$ is the *secant variety* of Y.

Proposition 3.5.

- *Let $Y \subset \mathbb{P}^{2n-1}$ be an irreducible linearly non-degenerate Legendrian variety. Then $\sigma_2(Y) = \mathbb{P}^{2n-1}$.*
- *Let $Y_1, Y_2 \subset \mathbb{P}^{2n-1}$ be two disjoint Legendrian subvarieties. Then $Y_1 * Y_2 = \mathbb{P}^{2n-1}$.*

Proof. If Y is irreducible, then this is proved in the course of proof of Prop. 17(2) in [LM07].
If Y_1 and Y_2 are disjoint, then the result follows from Lemma 3.4.

□

3.3 Divisors swept by broken lines

Following the idea of Wiśniewski [Wiś00] we introduce the locus of broken lines (or reducible conics, or chains of 2 lines) through x:

$$D_x := \bigcup_{y \in C_x} C_y.$$

Note that D_x is a closed subset of X as it can be interpreted as the image of projective variety $C_x^2 \subset X \times X$ under a proper map, which is the projection onto the last coordinate. By analogy to the case of lines consider also:

$$D^2 \subset X \times X$$
$$D^2 := \{(x, z) \mid \exists_{y \in C_x} \text{ s.t. } z \in C_y\},$$

i.e. D^2 is the projection of C^3 onto first and third coordinates. Thus again D^2 is a closed subset of the product. Set theoretically D_x is the fibre over x of (either of) the projection $D^2 \to X$ and if we consider D^2 as a reduced scheme, then we can assign to D_x the scheme structure of the fibre.
It follows immediately from the above discussion and Proposition 3.3, that every component of D_x has dimension at most $2n$ and every component of D^2 has dimension at most $4n + 1$. In fact the equality holds.

Theorem 3.6. *Let $x \in X$ be any point. Then the locus D_x is of pure codimension* 1.

Proof. Assume first that $x \in X$ is a general point. Recall, that $C_x^2 \subset X \times X$ has two projections:

$$\begin{array}{ccc} C_x^2 & \xrightarrow{\pi_2} & D_x \\ \downarrow{\scriptstyle \pi_1} & & \\ C_x & & \end{array}$$

Fix $(D_x)^\bullet$ to be an irreducible component of D_x. Then $(D_x)^\bullet$ is dominated by some component $(C_x^2)^\bullet$ of C_x^2. Dimension of $(C_x^2)^\bullet$ is equal to $2n$ by Proposition 3.3.
For $y \in C_x$ the fiber ${\pi_1}^{-1}(y) \subset C_x^2$ is equal to $\{y\} \times C_y$. In particular, by Theorem 3.1(ii) the fibers of π_1 have constant dimension n. Thus $(C_x^2)^\bullet$ is mapped onto an irreducible component $(C_x)^\bullet$ of C_x. Finally, let C' be an irreducible component of the preimage ${\pi_1}^{-1}(x)$ which is contained in $(C_x^2)^\bullet$. Note that C' can be identified with an irreducible component of C_x, because ${\pi_1}^{-1}(x) = \{x\} \times C_x$.
We claim that the projectivised tangent cone $\mathbb{P}\tau_x(D_x)^\bullet$ contains the join of two tangent cones

$$(\mathbb{P}\tau_x C') * (\mathbb{P}\tau_x (C_x)^\bullet) \subset \mathbb{P}F_x \subset \mathbb{P}T_x X.$$

The proof of the claim is a baby version of [HK05, Thm 3.11]. There however Hwang and Kebekus assume C_x is irreducible and thus their results do not neccessarily apply directly here. Let l_0 be a general line through x contained in C' and let l be a general line through x contained in $(C_x)^\bullet$. To prove the claim it is enough to show there exists a surface $S \subset D_x$ containing l_0 and l which is smooth at x, since in such a case $T_x S \subset \tau_x D_x$ and $\mathbb{P}T_x S$ is the line between $\mathbb{P}T_x l$ and $\mathbb{P}T_x l_0$.

We obtain S by varying l_0. Consider $\mathcal{H}_l \subset \mathcal{H}$ the parameter space for lines on X, which intersect l. By Theorem 3.1(iii) the space $\mathcal{H}_l$ comes with a projection $\xi\colon \mathcal{H}_l \dashrightarrow l$, which maps $l' \in \mathcal{H}_l$ to the intersection point of l and l', and which is well defined on an open subset containg all lines through x.
By generality of our choices, l_0 is a smooth point of $\mathcal{H}_l$ and ξ is submersive at l_0. In the neighbourhood of l_0 choose a curve $A \subset \mathcal{H}_l$ smooth at l_0 for which $\xi|_A$ is submersive at l_0. Then the locus in X of lines which are in A sweeps a surface $S \subset X$, which is smooth at x, contains l_0, and contains an open subset of l around x. Thus the claim is proved and:

$$(\mathbb{P}\tau_x C') * (\mathbb{P}\tau_x (C_x)^{\bullet}) \subset \mathbb{P}\tau_x (D_x)^{\bullet} \tag{3.7}$$

Now we claim that $F_x \subset \tau_x D_x$. For this purpose we separate two cases.
In the first case $C' = (C_x)^{\bullet}$. Then $\mathbb{P}\tau_x C'$ is non-degenerate by Theorem 3.1 and thus

$$(\mathbb{P}\tau_x C') * (\mathbb{P}\tau_x (C_x)^{\bullet}) = \sigma_2(\mathbb{P}\tau_x C') = \mathbb{P}(F_x)$$

by Proposition 3.5. Combining with (3.7) we obtain the claim.
In the second case C' and $(C_x)^{\bullet}$ are different components of C_x. Then by generality of x and by Theorem 3.1, the two tangent cones $(\mathbb{P}\tau_x C')$ and $(\mathbb{P}\tau_x (C_x)^{\bullet})$ are disjoint. Thus again

$$(\mathbb{P}\tau_x C') * (\mathbb{P}\tau_x (C_x)^{\bullet}) = \mathbb{P}(F_x)$$

by Proposition 3.5. Combining with (3.7) we obtain the claim.
Thus in any case for a general $x \in X$, every component of D_x has dimension at least $2n$. The dimension can only jump up at special points when one has a fibration, thus also at special points every component of D_x has dimension at least $2n$. Earlier we observed that $\dim D_x \leq 2n$, thus the theorem is proved. □

Proposition 3.8. *If X is the adjoint variety of G, and $x \in X$, then D_x is the hyperplane section of $X \subset \mathbb{P}(\mathfrak{g})$ perpendicular to x via the Killing form.*

Proof. Let $X = G/P$, where P is the parabolic subgroup preserving x. Notice, that D_x must be reduced (because D is reduced and D_x is a general fibre of D). Also D_x is P-invariant, because the set of lines is G invariant and D_x is determined by x and the geometry of lines on X. We claim, there is a unique P-invariant reduced divisor on X, and thus it must be the hyperplane section as in the statment of proposition.
So let Δ be a P-invariant divisor linearly equivalent to L^k for some $k \geq 0$. Also let ρ_Δ be a section of L^k which determines Δ. The module of sections $H^0(L^k)$ is an irreducible G-module by Borel-Weil theorem (see [Ser95]), with some highest weight ω. Since the Lie algebra $\mathfrak{p}$ of P contains all positive root spaces, by [FH91, Prop. 14.13] there is a unique 1-dimensional $\mathfrak{p}$-invariant submodule of $H^0(L^k)$, it is the highest weight space $H^0(L^k)_\omega$. So $\rho_\Delta \in H^0(L^k)_\omega$ and Δ is unique.

The hyperplane section of $X \subset \mathbb{P}(\mathfrak{g})$ perpendicular to x via the Killing form is a divisor in $|L|$, and it is P-invariant, and so are its multiples in $|L^k|$. So by the uniqueness Δ must be equal to k times this hyperplane section. Thus Δ is reduced if and only $k = 1$ and so D_x is the hyperplane section.

□

3.4 Tangent bundles restricted to lines

Let l be a line through a general point $y \in X$. Recall from [Keb05, Fact 2.3] that:

$$\begin{aligned} TX|_l &\simeq \mathcal{O}_l(2) \oplus \mathcal{O}_l(1)^{n-1} \oplus \mathcal{O}_l{}^{n-1} \oplus \mathcal{O}_l{}^2 \\ F|_l &\simeq \mathcal{O}_l(2) \oplus \mathcal{O}_l(1)^{n-1} \oplus \mathcal{O}_l{}^{n-1} \oplus \mathcal{O}_l(-1) \\ Tl &\simeq \mathcal{O}_l(2) \end{aligned}$$

and for general $z \in l$:

$$TC_z|_{l\setminus\{z\}} \simeq \mathcal{O}_l(2) \oplus \mathcal{O}_l(1)^{n-1}.$$

If $x \in X$ is a general point and $y \in C_x$ is a general point of any of the irreducible components of C_x and l is a line through y, then we want to express $TD_x|_l$ in terms of those splittings. In a neighbourhood of l the divisor D_x is swept by deformations l_t of $l = l_0$ such that l_t intersects C_x. By the standard deformation theory argument taking derivative of l_t by t at a point $z \in l$, we obtain that:

$$T_z D_x \supset \left\{ s(z) \in T_z X \mid \exists s \in H^0(TX|_l) \text{ s.t. } s(y) \in T_y C_x \right\} \tag{3.9}$$

Moreover, at a general point z we have equality in (3.9). If we mod out $TX|_l$ by the rank n positive bundle $(TX|_l)^{>0} := \mathcal{O}_l(2) \oplus \mathcal{O}_l(1)^{n-1}$, then we are left with a trivial bundle $\mathcal{O}_l{}^{n+1}$. Thus, since by Theorem 3.6 the dimension of $T_z D_x = 2n$ for general $z \in l$, the vector space $T_y C_x$ must be transversal to $(TX|_l)^{>0}$ at y. In particular, if $z \neq y$, then dimension of the right hand side in (3.9) is $2n$ and thus (3.9) is an equality for each point $z \in l$, such that z is a smooth point of D_x.
We conclude:

Proposition 3.10. *Let $x \in X$ be a general point and $y \in C_x$ be a general point of any of the irreducible components of C_x and l be any line through y. Then there exists a subbundle $\Gamma \subset TX|_l$ such that:*

$$\begin{aligned} \Gamma &= \mathcal{O}_l(2) \oplus \mathcal{O}_l(1)^{n-1} \oplus \mathcal{O}_l{}^n, \\ \Gamma \cap F|_l &= \mathcal{O}_l(2) \oplus \mathcal{O}_l(1)^{n-1} \oplus \mathcal{O}_l{}^{n-1} = (F|_l)^{\geq 0} \end{aligned}$$

and if $z \in l$ is a smooth point of D_x, then $T_z D_x = \Gamma_z$.

□

4 Duality

An effective divisor Δ on X is an element of divisor group (and thus a positive integral combination of codimension 1 subvarieties of X) and also a point in the projective space $\mathbb{P}(H^0\mathcal{O}_X(\Delta))$ or a hyperplane in $\mathbb{P}(H^0\mathcal{O}_X(\Delta)^*)$. In this section we will constantly interchange these three interpretations of Δ. In order to avoid confusion we will write:

- Δ^{div} to mean the divisor on X;
- $\Delta^{\mathbb{P}}$ to mean the point in $\mathbb{P}(H^0\mathcal{O}_X(\Delta))$ or in a fixed linear subsystem.
- $\Delta^{\mathbb{P}\perp}$ to mean the hyperplane in $\mathbb{P}(H^0\mathcal{O}_X(\Delta)^*)$ or in dual of the fixed subsystem.

In §3.3 we have defined $D \subset X \times X$, which we now view as a family of divisors on X parametrised by X. Since the Picard group of X is discrete and X is smooth and connected, it follows that all the divisors D_x are linearly equivalent. Thus let $E \simeq L^{\otimes k}$ be the line bundle $\mathcal{O}_X(D_x)$. Consider the following vector space $\langle D \rangle \subset H^0(E)$:

$$\langle D \rangle := \operatorname{span}\{s_x : x \in X\} \text{ where } s_x \text{ is a section of } E \text{ vanishing on } D_x.$$

Hence $\mathbb{P}\langle D \rangle$ is the linear system spanned by all the D_x.
Further, consider the map

$$\phi : X \to \mathbb{P}\langle D \rangle^*$$

determined by the linear system $\langle D \rangle$, i.e. mapping point $x \in X$ to the hyperplane in $\mathbb{P}\langle D \rangle$ consisting of all divisors containing x.

Remark 4.1. Note that ϕ is regular, since for every $x \in X$ there exists $w \in X$, such that $x \notin D_w$ (or equivalently, $w \notin D_x$).

Since E is ample, it must intersect every curve in X and hence ϕ does not contract any curve. Therefore ϕ is finite to one.

Proposition 4.2. *If X is an adjoint variety, then $k = 1$, i.e. $E \simeq L$. If $k = 1$ and the automorphism group of X is reductive, then X is isomorphic to an adjoint variety.*

Proof. If X is the adjoint variety of G, and $x \in X$, then D_x is the hyperplane section of $X \subset \mathbb{P}(\mathfrak{g})$ by Proposition 3.8.
If $k = 1$ and the automorphism group of X is reductive, since ϕ is finite to one, we can apply Beauville Theorem [Bea98]. Thus X is isomorphic to an adjoint variety.

□

4.1 Dual map

In algebraic geometry it is standard to consider maps determined by linear systems (such as ϕ defined above). However in our situation, we also have another map determined by the family of divisors D. Namely:

$$\psi\colon X \to \mathbb{P}\langle D\rangle$$
$$x \mapsto {D_x}^{\mathbb{P}}.$$

So let $\mathcal{S} \subset \mathcal{O}_X \otimes \langle D\rangle^* \simeq X \times \langle D\rangle^*$ be the pullback under ϕ of the universal hyperplane bundle, i.e. the corank 1 subbundle such that the fibre of $\mathcal{S}$ over x is ${D_x}^{\mathbb{P}\perp} \subset \langle D\rangle^*$. We note that $\mathbb{P}(\mathcal{S})$ is both a projective space bundle on X and also it is a divisor on $X \times \mathbb{P}\langle D\rangle^*$. Also $D = (\mathrm{id}_X \times \phi)^* \mathbb{P}(\mathcal{S})$ as divisors.
We can also consider the line bundle dual to the cokernel of $\mathcal{S} \to \mathcal{O}_X \otimes \langle D\rangle^*$, i.e. the subbundle $\mathcal{S}^\perp \subset \mathcal{O}_X \otimes \langle D\rangle$. This line subbundle determines section $X \to X \times \mathbb{P}\langle D\rangle$, where $x \mapsto (x, {D_x}^{\mathbb{P}})$. So ψ is the composition of the section and the projection:

$$X \to X \times \mathbb{P}\langle D\rangle \to \mathbb{P}\langle D\rangle.$$

Every map to a projective space is determined by some linear system. We claim the ψ is determined by $\langle D\rangle$, precisely the system that defines ϕ and thus that there is a natural linear isomorphism between $\mathbb{P}\langle D\rangle$ and $\mathbb{P}\langle D\rangle^*$.

Proposition 4.3. *We have $\psi^* \mathcal{O}_{\mathbb{P}\langle D\rangle}(1) \simeq E$ and the linear system cut out by hyperplanes*

$$\psi^* H^0\left(\mathcal{O}_{\mathbb{P}\langle D\rangle}(1)\right) := \left\{\psi^* s : s \in \langle D\rangle^*\right\} \subset H^0(E)$$

is equal to $\langle D\rangle$.

Proof. For fixed $x \in X$ let $\phi(x)^\perp \subset \mathbb{P}\langle D\rangle$ be the hyperplane dual to $\phi(x) \in \mathbb{P}\langle D\rangle^*$. To prove the proposition it is enough to prove

$$\psi^*(\phi(x)^\perp) = {D_x}^{div}. \tag{4.4}$$

Since we have the following symmetry property of D:

$$x \in D_y \iff y \in D_x,$$

the set theoretic version of (4.4) follows easily:

$$y \in \psi^*(\phi(x)^\perp) \iff \psi(y) \in \phi(x)^\perp \iff {D_y}^{\mathbb{P}\perp} \ni \phi(x) \iff D_y \ni x.$$

However, in order to prove the equality of divisors in (4.4) we must do a bit more of gymnastics, which translates the equivalences above into local equations. The details are below.
The pull back of $\phi(x)^\perp$ by the projection $X \times \mathbb{P}\langle D\rangle \to \mathbb{P}\langle D\rangle$ is just $X \times \phi(x)^\perp$. Then the pull-back of the product by the section $X \to X \times \mathbb{P}\langle D\rangle$ associated

to $\mathcal{S}^\perp$ is just the subscheme of X defined by $\left\{y \in X \mid (\mathcal{S}^\perp)_y \subset \phi(x)^\perp\right\}$ (locally, this is just a single equation: the spanning section of $\mathcal{S}^\perp$ satisfies the defining equation of $\phi(x)^\perp$). But this is clearly equal to the dual equation $\{y \mid \mathbb{P}(\mathcal{S}_y) \ni \phi(x)\}$. If we let ρ_x be the section

$$\begin{aligned} \rho_x \colon X &\to X \times X \\ \rho_x(y) &:= (y, x) \end{aligned}$$

then we have:

$$\psi^*(\phi(x)^\perp) = {\rho_x}^* \circ (\mathrm{id}_X \times \phi)^*(\mathbb{P}(\mathcal{S})) = {\rho_x}^*(D) = {D_x}^{div}$$

as claimed.

□

Thus we have a canonical linear isomorphism $f \colon \mathbb{P}\langle D\rangle^* \to \mathbb{P}\langle D\rangle$ giving rise to the following commutative diagram:

$$\begin{array}{ccc} & & \mathbb{P}\langle D\rangle^* \\ & \overset{\phi}{\nearrow} & \\ X & & \Big\downarrow \simeq \\ & \underset{\psi}{\searrow} & \\ & & \mathbb{P}\langle D\rangle. \end{array} \tag{4.5}$$

We will denote the underlying vector space isomorphism $\langle D\rangle^* \to \langle D\rangle$ (which is unique up to scalar) with the same letter f. The choice of f combined with the canonical pairing $\langle D\rangle \times \langle D\rangle^* \to \mathbb{C}$, determines a non-degenerate bilinear form $B : \langle D\rangle \times \langle D\rangle \to \mathbb{C}$, with the following property:

$$B(\phi(x), \phi(y)) = 0 \iff (x, y) \in D \iff x \in D_y \iff y \in D_x. \tag{4.6}$$

Proposition 4.7. *If X is the adjoint variety of G, then $\langle D\rangle = H^0(L) \simeq \mathfrak{g}$ and B is (up to scalar) the Killing form on $\mathfrak{g}$.*

Proof. Follows immediately from Proposition 3.8 and Equation 4.6.

□

Corollary 4.8. *$\phi(x) = \phi(y)$ if and only if $D_x = D_y$.*

Proof. It is immediate from the definition of ψ and from Diagram (4.5).

□

4.2 Symmetry

Note that B has the property that for $x \in X$,

$$B(\phi(x), \phi(x)) = 0$$

(because $x \in D_x$).

Proposition 4.9. *The bilinear form B is either symmetric or skew-symmetric.*

Proof. Consider two linear maps $\langle D\rangle \to \langle D\rangle^*$:

$$\alpha(v) := B(v,\cdot) \quad \text{and} \quad \beta(v) := B(\cdot, v).$$

If $v = \phi(x)$ for some $x \in X$, then

$$\ker\big(\alpha(v)\big) = \operatorname{span}\Big(\ker\big(\alpha(v)\big) \cap \phi(X)\Big) = \operatorname{span}\big(\phi(D_x)\big)$$

and analogously $\ker(\beta(v)) = \operatorname{span}(\phi(D_x))$. So $\ker(\alpha(v)) = \ker(\beta(v))$ and hence $\alpha(v)$ and $\beta(v)$ are proportional. Therefore there exists a function $\lambda : X \to \mathbb{C}$ such that:

$$\lambda(x)\alpha(\phi(x)) = \beta(\phi(x)).$$

So for every $x, y \in X$ we have:

$$B(\phi(x),\phi(y)) = \lambda(x)B(\phi(y),\phi(x)) = \lambda(x)\lambda(y)B(\phi(x),\phi(y))$$

and hence:

$$\forall (x,y) \in X \times X \setminus D \qquad \lambda(x)\lambda(y) = 1.$$

Taking three different points we see that λ is constant and $\lambda \equiv \pm 1$. Therefore $\pm\alpha(\phi(x)) = \beta(\phi(x))$ and by linearity this extends to $\pm\alpha = \beta$ so B is either symmetric or skew-symmetric as stated in the proposition.

□

Example 4.10. If X is one of the adjoint varieties, then B is symmetric (because the Killing form is symmetric).

Remark 4.11. Consider $\mathbb{P}^{2n+1}$ with a contact structure arising from a symplectic form ω on $\mathbb{C}^{2n+2}$. Recall, that this homogeneous contact Fano manifold does not satisfy our assumptions, namely, its Picard group is not generated by the equivalence class of L — in this case $L \simeq \mathcal{O}_{\mathbb{P}^{2n+1}}(2)$. However, Wiśniewski in [Wiś00] considers also this generalised situation and defines D_x to be the divisor swept by contact conics (i.e. curves C with degree of $L|_C = 2$) tangent to the contact distribution F. Then for the projective space D_x is just the hyperplane perpendicular to x with respect to ω. And thus in this case $\langle D\rangle = H^0\left(\mathcal{O}_{\mathbb{P}^{2n+1}}(1)\right)$ and the bilinear form B defined from such family of divisors would be proportional to ω, hence skew-symmetric.

Proof of Theorem 1.3. D_x is a divisor by Theorem 3.6. ϕ is regular by Remark 4.1. ψ is regular by (4.5). The non-degenerate bilinear form B is constructed in §4.1. It is either symmetric or skew-symmetric by Proposition 4.9. In the adjoint case B is the Killing form by Proposition 4.7.

□

COROLLARY 4.12. *If B is symmetric, then $\psi(X) \subset \mathbb{P}\langle D\rangle$ is contained in the quadric $B(v,v) = 0$.*

COROLLARY 4.13. *If $x \in X$, then $\psi(C_x)$ is contained in a linear subspace of dimension at most $\left\lfloor \frac{\dim \langle D\rangle}{2} \right\rfloor$.*

PROOF. If $y, z \in C_x$, then $z \in D_y$, so $B(\psi(y), \psi(z)) = 0$. Therefore $\mathrm{span}(\psi(C_x))$ is an isotropic linear subspace, which cannot have dimension bigger than $\left\lfloor \frac{\dim \langle D\rangle}{2} \right\rfloor$.

□

5 GRADING

Suppose $X \subset \mathbb{P}\mathfrak{g}$ is the adjoint variety of G. Assume further that a maximal torus and an order of roots in $\mathfrak{g}$ has been chosen, then $\mathfrak{g}$ has a natural grading (see [LM02, §6.1]):

$$\mathfrak{g} = \mathfrak{g}_{-2} \oplus \mathfrak{g}_{-1} \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_2$$

where:

(i) $\mathfrak{g}_0 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_2$ is the parabolic subalgebra $\mathfrak{p}$ of X.

(ii) $\mathfrak{g}_0$ is the maximal reductive subalgebra of $\mathfrak{p}$.

(iii) for all $i \in \{-2, -1, 0, 1, 2\}$ the vector space $\mathfrak{g}_i$ is a $\mathfrak{g}_0$-module.

(iv) $\mathfrak{g}_2$ is the 1-dimensional highest root space,

(v) $\mathfrak{g}_{-2}$ is the 1-dimensional lowest root space.

(vi) The restriction of the Killing form to each $\mathfrak{g}_2 \oplus \mathfrak{g}_{-2}$, $\mathfrak{g}_1 \oplus \mathfrak{g}_{-1}$ and $\mathfrak{g}_0$ is non-degenerate, and the Killing form $B(\mathfrak{g}_i, \mathfrak{g}_j)$ is identically zero for $i \neq -j$.

(vii) The Lie bracket on $\mathfrak{g}$ respects the grading, $[\mathfrak{g}_i, \mathfrak{g}_j] \subset \mathfrak{g}_{i+j}$ (where $\mathfrak{g}_k = 0$ for $k \notin \{-2, -1, 0, 1, 2\}$).

In fact the grading is determined by $\mathfrak{g}_{-2}$ and $\mathfrak{g}_2$ together with the geometry of X only. So let X be as in Notation 2.1 and let x and w be two general points of X. Define the following subspaces of $\langle D\rangle$:

- $\langle D\rangle_2$ to be the 1-dimensional subspace $\psi(x)$;
- $\langle D\rangle_{-2}$ to be the 1-dimensional subspace $\psi(w)$;
- $\langle D\rangle_1$ to be the linear span of affine cone of $\psi(C_x \cap D_w)$;
- $\langle D\rangle_{-1}$ to be the linear span of affine cone of $\psi(C_w \cap D_x)$;

- $\langle D\rangle_0$ to be the vector subspace of $\langle D\rangle$, whose projectivisation is:

$$\bigcap_{y\in C_x\cup C_w} f({D_y}^{\mathbb{P}\perp})$$

In the homogeneous case this is precisely the grading of $\mathfrak{g}$.

Proof of Theorem 1.4. First note that the classes of the 1-dimensional linear subspaces $\mathfrak{g}_2$ and $\mathfrak{g}_{-2}$ are both in X (as points in $\mathbb{P}\mathfrak{g}$). Moreover, they are a pair of general points, because the action of the parabolic subgroup $P < G$ preserves $\mathfrak{g}_2$ and moves freely $\mathfrak{g}_{-2}$. This is because $\hat{T}_{[\mathfrak{g}_{-2}]}X = [\mathfrak{g}_{-2}, \mathfrak{g}] = [\mathfrak{g}_{-2}, \mathfrak{p}]$. So fix $x = [\mathfrak{g}_2]$ and $w = [\mathfrak{g}_{-2}]$. We claim the linear span of C_x (respectively C_w) is just $\mathfrak{g}_2 \oplus \mathfrak{g}_1$ (respectively $\mathfrak{g}_{-2} \oplus \mathfrak{g}_{-1}$). To see that, we observe the lines on X through x are contained in the intersection of X and the projective tangent space $\mathbb{P}(\hat{T}_x X) \subset \mathbb{P}(\mathfrak{g})$. In fact this intersection is equal to C_x: if $y \neq x$ is a point of the intersection, then the line in $\mathbb{P}\mathfrak{g}$ through x and y intersects X with multiplicity at least 3, but X is cut out by quadrics (see for instance [Pro07, §10.6.6]), so this line must be contained in X. Also C_x is non-degenerate in $\mathbb{P}(\hat{F}_x) \subset \mathbb{P}(\hat{T}_x X)$. However $\hat{F}_x$ is a $\mathfrak{p}$-invariant hyperplane in $\mathbb{P}(\hat{T}_x X)$ and the unique $\mathfrak{p}$-invariant hyperplane in

$$\hat{T}_x X = [\mathfrak{g}, \mathfrak{g}_2] = [\mathfrak{g}_{-2}, \mathfrak{g}_2] \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_2$$

is

$$\hat{F}_x = [\mathfrak{g}_{-1} \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_2, \mathfrak{g}_2] = \mathfrak{g}_1 \oplus \mathfrak{g}_2.$$

Further we have seen in Proposition 3.8 that D_x (respectively D_w) is the intersection of $\mathbb{P}({\mathfrak{g}_2}^{\perp_B}) = \mathbb{P}(\mathfrak{g}_2 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_{-1})$ and X (respectively $\mathbb{P}(\mathfrak{g}_{-2} \oplus \mathfrak{g}_{-1} \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_1)$ and X). Equivalently, $f({D_x}^{\mathbb{P}\perp}) = \mathbb{P}(\mathfrak{g}_2 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_{-1})$. Thus:

$$C_x \cap D_w = C_x \cap f({D_w}^{\mathbb{P}\perp}) = C_x \cap \mathbb{P}(\mathfrak{g}_{-2} \oplus \mathfrak{g}_{-1} \oplus \mathfrak{g}_0 \oplus \mathfrak{g}_1) = C_x \cap \mathbb{P}(\mathfrak{g}_1).$$

$C_x \cap \mathbb{P}(\mathfrak{g}_1)$ is non-degenerate in $\mathbb{P}(\mathfrak{g}_1)$, thus $\langle D\rangle_1 = \mathfrak{g}_1$ and analogously $\langle D\rangle_{-1} = \mathfrak{g}_{-1}$.
It remains to prove $\langle D\rangle_0 = \mathfrak{g}_0$.

$$\begin{aligned}
\mathbb{P}\langle D\rangle_0 &= \bigcap_{y\in C_x\cup C_w} f({D_z}^{\mathbb{P}\perp}) \\
&= (C_x \cup C_w)^{\perp_B} \\
&= \mathbb{P}(\mathfrak{g}_2 \oplus \mathfrak{g}_1 \oplus \mathfrak{g}_{-1} \oplus \mathfrak{g}_{-2})^{\perp_B} \\
&= \mathbb{P}(\mathfrak{g}_0).
\end{aligned}$$

□

We also note the following lemma in the homogeneous case:

Lemma 5.1. *If X is the adjoint variety of G, then*

$$X \cap \mathbb{P}(\mathfrak{g}_1) \subset C_x$$

where x is the point of projective space corresponding to $\mathfrak{g}_2$.

Proof. Suppose $y \in X \cap \mathbb{P}\mathfrak{g}_1$ and let $l \subset \mathbb{P}\mathfrak{g}$ be the line through x and y. Note that $l \subset \mathbb{P}(\mathfrak{g}_1 \oplus \mathfrak{g}_2)$. Since $\mathfrak{g}_1 \oplus \mathfrak{g}_2 \subset [\mathfrak{g}, \mathfrak{g}_2] = \hat{T}_x X$, hence $l \cap X$ has multiplicity at least 2 at x. Thus $l \cap X$ has degree at least 3 and since X is cut out by quadrics, l is contained in X.

□

6 Cointegrable subvarieties

Definition 6.1. A subvariety $\Delta \subset X$ is *F-cointegrable* if $T_x\Delta \cap F_x \subset F_x$ is a coisotropic subspace for general point x of each irreducible component of Δ.

Note that this is equivalent to the definition given in [Bucz09, §E.4] — this follows from the local description of the symplectic form on the symplectisation of the contact manifold (see [Bucz09, (C.15)]).
Clearly, every codimension 1 subvariety of X is F-cointegrable.
Assume $\Delta \subset X$ is a subvariety of pure dimension, which is F-cointegrable and let Δ_0 be the locus where $T_x\Delta \cap F_x \subset F_x$ is a coisotropic subspace of dimension $\dim \Delta - 1$. We define the Δ-*integrable distribution* $\Delta^{\perp}$ to be the distribution defined over Δ_0 by:

$$\Delta^{\perp}{}_x := (T_x\Delta \cap F_x)^{\perp_{d\theta}} \subset F_x$$

We say an irreducible subvariety $A \subset X$ is Δ-*integral* if $A \subset \Delta$, $A \cap \Delta_0 \neq \emptyset$, and $TA \subset \Delta^{\perp}$ over the smooth points of $A \cap \Delta_0$.

Lemma 6.2. *Let A_1 and A_2 be two irreducible Δ-integral subvarieties. Assume $\dim A_1 = \dim A_2 = \operatorname{codim}_X \Delta$. Then either $A_1 = A_2$ or $A_1 \cap A_2 \subset \Delta \setminus \Delta_0$.*

□

Theorem 6.3. *Consider a general point $x \in X$. Then:*

(i) D_x (as reduced, but possibly not irreducible subvariety of X) is F-cointegrable.

(ii) For general y in any of the irreducible components of C_x all lines through y are D_x-integral.

(iii) For general z in any of the irreducible components of D_x the intersection $C_x \cap C_z$ is a unique point and the chain of two lines connecting x to z is unique.

Proof. Part (i) is immediate, since D_x is a divisor, by Theorem 3.6.
To prove part (ii) let l be a line through y. Then by Proposition 3.10:

$$T_z D_x \cap F_z = (F|_l)^{\geq 0}$$

and for general $z \in l$ we have $(T_z D_x \cap F_z)^{\perp_{d\theta_z}} \subset F_z$ is the $\mathcal{O}(2)$ part, i.e. the part tangent to l. So l is D_x-integral as claimed.
To prove (iii), let $U \subset X$ be an open dense subset of points $u \in X$ where two different lines through u do not share the tangent direction and do not meet in any other point. Note that since x is a general point, $x \in U$ and thus each irreducible component of C_x and D_x intersects U. Thus generality of z implies that $z \in U$ and thus each irreducible component of C_z and D_z intersects U. Also $C_x \cap C_z$ intersects U. So fix $y \in C_x \cap C_z \cap U$.
By (ii) and Lemma 6.2 the line l_z through z which intersects C_x is unique. In the same way let l_x be the unique line through x intersecting C_z. Thus

$$C_x \cap C_z = l_x \cap l_z.$$

In particular, $y \in l_x \cap l_z$. But since $y \in U$ the intersection $l_x \cap l_z$ is just one point and therefore:

$$C_x \cap C_z = \{y\}.$$

□

As a consequence of part (iii) of the theorem the surjective map $\pi_{13} \colon C^3 \to D$ is birational. Thus consider the inverse rational map $D \dashrightarrow C^3$ and compose it with the projection on the middle coordinate $\pi_2 : C^3 \to X$. We define the composition to be the *bracket map*:

$$[\cdot,\cdot]^D \colon D \dashrightarrow C^3 \xrightarrow{\pi_2} X.$$

In this setting, for $(x, z) \in D$, one has $[x, z]^D = y = C_x \cap C_z$, whenever the intersection is just one point.

Theorem 6.4. *If X is the adjoint variety of G, then the bracket map defined above agrees with the Lie bracket on $\mathfrak{g}$, in the following sense: Let $\xi, \zeta \in \mathfrak{g}$ and set $\eta := [\xi, \zeta]$ (the Lie bracket on $\mathfrak{g}$). Denote by x, y and z the projective classes in $\mathbb{P}\mathfrak{g}$ of ξ, η and ζ respectively. If $x \in D_z$ and $\eta \neq 0$, then the bracket map satisfies $[x, z]^D = y$.*

Proof. It is enough to prove the statement for a general pair $(x, z) \in D$. Suppose further $w \in C_z$ is a general point. Then the pair $(x, w) \in X \times X$ is a general pair. Thus by Theorem 1.4, we may assume $\xi \in \mathfrak{g}_2$ and $\zeta \in \mathfrak{g}_{-1}$. The restriction of the Lie bracket to $[\xi, \mathfrak{g}_{-1}]$ determines an isomorphism $\mathfrak{g}_{-1} \to \mathfrak{g}_1$ of $\mathfrak{g}_0$-modules. In particular the minimal orbit $X \cap \mathbb{P}\mathfrak{g}_{-1}$ is mapped onto $X \cap \mathbb{P}\mathfrak{g}_1$ under this isomorphism. In particular $y \in X \cap \mathbb{P}\mathfrak{g}_1 \subset C_x$ (see Lemma 5.1). Analogously $y \in C_z$, so $y \in C_x \cap C_z$.

□

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$\mathbb{Q}$-Fano Threefolds of Large Fano Index, I

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Abstract. We study $\mathbb{Q}$-Fano threefolds of large Fano index. In particular, we prove that the maximum possible Fano index is attained only by the weighted projective space $\mathbb{P}(3,4,5,7)$.

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1. Introduction

The Fano index of a smooth Fano variety X is the maximal integer $\mathrm{q}(X)$ that divides the anti-canonical class in the Picard group $\mathrm{Pic}(X)$ [IP99]. It is well-known [KO73] that $\mathrm{q}(X) \le \dim X + 1$. Moreover, $\mathrm{q}(X) = \dim X + 1$ if and only if X is a projective space and $\mathrm{q}(X) = \dim X$ if and only if X is a quadric hypersurface. In this paper we consider generalizations of Fano index for the case of singular Fanos admitting terminal singularities.

A normal projective variety X is called *Fano* if some positive multiple $-nK_X$ of its anti-canonical Weil divisor is Cartier and ample. Such X is called a $\mathbb{Q}$-*Fano variety* if it has only terminal $\mathbb{Q}$-factorial singularities and its Picard number is one. This class of Fano varieties is important because they appear naturally in the Minimal Model Program.

For a singular Fano variety X the Fano index can be defined in different ways. For example, we can define

$$\mathrm{qW}(X) := \max\{q \mid -K_X \sim qA, \quad A \text{ is a Weil } \mathbb{Q}\text{-Cartier divisor}\},$$

$$\mathrm{q}\mathbb{Q}(X) := \max\{q \mid -K_X \sim_{\mathbb{Q}} qA, \quad A \text{ is a Weil } \mathbb{Q}\text{-Cartier divisor}\}.$$

If X has at worst log terminal singularities, then the Picard group $\mathrm{Pic}(X)$ and Weil divisor class group $\mathrm{Cl}(X)$ are finitely generated and $\mathrm{Pic}(X)$ is torsion free (see e.g. [IP99, §2.1]). Moreover, the numerical equivalence of $\mathbb{Q}$-Cartier

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divisors coincides with $\mathbb{Q}$-linear one. This implies, in particular, that the Fano indices $\mathrm{qW}(X)$ and $\mathrm{q}\mathbb{Q}(X)$ defined above are positive integers. If X is smooth, these numbers coincide with the Fano index $\mathrm{q}(X)$ defined above. Note also that $\mathrm{q}\mathbb{Q}(X) = \mathrm{qW}(X)$ if the group $\mathrm{Cl}(X)$ is torsion free.

Theorem 1.1 ([Suz04]). *Let X be a $\mathbb{Q}$-Fano threefold. Then* $\mathrm{qW}(X) \in \{1, \dots, 11, 13, 17, 19\}$. *All these values, except possibly for* $\mathrm{qW}(X) = 10$, *occur. Moreover, if* $\mathrm{qW}(X) = 19$, *then the types of non-Gorenstein points and Hilbert series of X coincide with that of* $\mathbb{P}(3, 4, 5, 7)$.

It can be easily shown (see proof of Proposition 3.6) that the index $\mathrm{q}\mathbb{Q}(X)$ takes values in the same set $\{1, \dots, 11, 13, 17, 19\}$. Thus one can expect that $\mathbb{P}(3, 4, 5, 7)$ is the only example of $\mathbb{Q}$-Fano threefolds with $\mathrm{q}\mathbb{Q}(X) = 19$. In general, we expect that Fano varieties with extremal properties (maximal degree, maximal Fano index, etc.) are quasihomogeneous with respect to an action of some connected algebraic group. This is supported, for example, by the following facts:

Theorem 1.2 ([Pro05], [Pro07]).
(i) *Let X be a $\mathbb{Q}$-Fano threefold. Assume that X is not Gorenstein. Then $-K_X^3 \le 125/2$ and the equality holds if and only if X is isomorphic to the weighted projective space* $\mathbb{P}(1^3, 2)$.
(ii) *Let X be a Fano threefold with canonical Gorenstein singularities. Then $-K_X^3 \le 72$ and the equality holds if and only if X is isomorphic to* $\mathbb{P}(1^3, 3)$ *or* $\mathbb{P}(1^2, 6, 4)$.

The following proposition is well-known (see, e.g., [BB92]). It is an easy exercise for experts in toric geometry.

Proposition 1.3. *Let X be a toric $\mathbb{Q}$-Fano 3-fold. Then X is isomorphic to either* $\mathbb{P}^3$, $\mathbb{P}^3/\boldsymbol{\mu}_5(1, 2, 3, 4)$, *or one of the following weighted projective spaces:*

$$\mathbb{P}(1^3, 2),\ \ \mathbb{P}(1^2, 2, 3),\ \ \mathbb{P}(1, 2, 3, 5),\ \ \mathbb{P}(1, 3, 4, 5),\ \ \mathbb{P}(2, 3, 5, 7),\ \ \mathbb{P}(3, 4, 5, 7).$$

We characterize the weighted projective spaces above in terms of Fano index. The following is the main result of this paper.

Theorem 1.4. *Let X be a $\mathbb{Q}$-Fano threefold. Then* $\mathrm{q}\mathbb{Q}(X) \in \{1, \dots, 11, 13, 17, 19\}$.

(i) *If* $\mathrm{q}\mathbb{Q}(X) = 19$, *then* $X \simeq \mathbb{P}(3, 4, 5, 7)$.
(ii) *If* $\mathrm{q}\mathbb{Q}(X) = 17$, *then* $X \simeq \mathbb{P}(2, 3, 5, 7)$.
(iii) *If* $\mathrm{q}\mathbb{Q}(X) = 13$ *and* $\dim |-K_X| > 5$, *then* $X \simeq \mathbb{P}(1, 3, 4, 5)$.
(iv) *If* $\mathrm{q}\mathbb{Q}(X) = 11$ *and* $\dim |-K_X| > 10$, *then* $X \simeq \mathbb{P}(1, 2, 3, 5)$.
(v) $\mathrm{q}\mathbb{Q}(X) \ne 10$.
(vi) *If* $\mathrm{q}\mathbb{Q}(X) \ge 7$ *and there are two effective Weil divisors* $A \ne A_1$ *such that* $-K_X \sim_{\mathbb{Q}} \mathrm{q}\mathbb{Q}(X)A \sim_{\mathbb{Q}} \mathrm{q}\mathbb{Q}(X)A_1$, *then* $X \simeq \mathbb{P}(1^2, 2, 3)$.
(vii) *If* $\mathrm{qW}(X) = 5$ *and* $\dim |-\frac{1}{5}K_X| > 1$, *then* $X \simeq \mathbb{P}(1^3, 2)$.

Note that in cases (iii) and (iv) assumptions about $|-K_X|$ are really needed. Indeed, there are examples of non-toric $\mathbb{Q}$-Fano threefolds with $\mathrm{q}\mathbb{Q}(X) = 13$ and 11.

Example 1.5 ([BS07], see also Proposition 3.6). Let $X = X_d \subset \mathbb{P}(a_1, \dots, a_5)$ be a general hypersurface of degree d. Assume that X is a $\mathbb{Q}$-Fano with $\mathrm{q}\mathbb{Q}(X) \geq 10$ and such that $\mathscr{O}_{\mathbb{P}}(1)|_X$ is a primitive element of $\mathrm{Cl}(X)$, then X is one of the following:

(i) $X = X_{12} \subset \mathbb{P}(1, 4, 5, 6, 7)$, $\mathrm{q}\mathbb{Q}(X) = 11$, $\dim|-K_X| = 10$;
(ii) $X = X_{10} \subset \mathbb{P}(2, 3, 4, 5, 7)$, $\mathrm{q}\mathbb{Q}(X) = 11$, $\dim|-K_X| = 8$;
(iii) $X \simeq X_{12} \subset \mathbb{P}(3, 4, 5, 6, 7)$, $\mathrm{q}\mathbb{Q}(X) = 13$, $\dim|-K_X| = 5$.

In the proof we follow the use some techniques developed in our previous paper [Pro07]. By Proposition 1.3 it is sufficient to show that our $\mathbb{Q}$-Fano X is toric. First, as in [Suz04], we apply the orbifold Riemann-Roch formula to find all the possibilities for the numerical invariants of X. In all cases there is some special element $S \in |-K_X|$ having four irreducible components. This S should be a toric boundary, if X is toric. Further, we use birational transformations like Fano-Iskovskikh "double projection" [IP99] (see [Ale94] for the $\mathbb{Q}$-Fano version). Typically the resulting variety is a Fano-Mori fiber space having "simpler" structure. In particular, its Fano index is large if this variety is a $\mathbb{Q}$-Fano. By using properties of our "double projection" we can show that the pair (X, S) is log canonical (LC). Then, in principle, the assertion follows by Shokurov's toric conjecture [McK01]. We prefer to propose an alternative, more explicit proof. In fact, the image of X under "double projection" is a toric variety and the inverse map preserves the toric structure. In the last section we describe Sarkisov links between toric $\mathbb{Q}$-Fanos that start with blow ups of *singular* points.

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2. Preliminaries, the orbifold Riemann-Roch formula and its applications

Notation. Throughout this paper, we work over the complex number field $\mathbb{C}$. We employ the following standard notation:
$\sim$ denotes linear equivalence;
$\sim_{\mathbb{Q}}$ denotes $\mathbb{Q}$-linear equivalence.
Let E be a rank one discrete valuation of the function field $\mathbb{C}(X)$ and let D be a $\mathbb{Q}$-Cartier divisor on X. $a(E, D)$ denotes the discrepancy of E with respect to a boundary D. Let $f \colon \tilde{X} \to X$ be a birational morphism such that E appears as a prime divisor on $\tilde{X}$. Then $\mathrm{ord}_E(D)$ denotes the coefficient of E in f^*D.

2.1. The orbifold Riemann-Roch formula [Rei87]. Let X be a threefold with terminal singularities and let D be a Weil $\mathbb{Q}$-Cartier divisor on X. Let $\mathbf{B} = \{(r_P, b_P)\}$ be the basket of singular points of X [Mor85a], [Rei87]. Here each pair (r_P, b_P) correspond to a point $P \in \mathbf{B}$ of type $\frac{1}{r_P}(1,-1,b_P)$. For brevity, describing a basket we will list just indices of singularities, i.e., we will write $\mathbf{B} = \{r_P\}$ instead of $\mathbf{B} = \{(r_P, b_P)\}$. In the above situation, the Riemann-Roch formula has the following form

$$\chi(D) = \frac{1}{12} D\cdot(D-K_X)\cdot(2D-K_X) + \\ + \frac{1}{12} D\cdot c_2 + \sum_{P\in\mathbf{B}} c_P(D) + \chi(\mathscr{O}_X), \tag{2.2}$$

where

$$c_P(D) = -i_P\frac{r_P^2-1}{12r_P} + \sum_{j=1}^{i_P-1}\frac{\overline{b_P j}(r_P-\overline{b_P j})}{2r_P}.$$

Clearly, computing $c_P(D)$, we always may assume that $1 \le b_P \le r_P/2$.

2.3. Now let X be a Fano threefold with terminal singularities, let $q := \mathrm{q}\mathbb{Q}(X)$, and let A be an ample Weil $\mathbb{Q}$-Cartier divisor on X such that $-K_X \sim_{\mathbb{Q}} qA$. By (2.2) we have

$$\chi(tA) = \chi(\mathscr{O}_X) + \frac{t(q+t)(q+2t)}{12}A^3 + \frac{tA\cdot c_2}{12} + \sum_{P\in\mathbf{B}} c_P(tA), \tag{2.4}$$

where $\chi(\mathscr{O}_X) = 1$ and

$$c_P(tA) = -i_{P,t}\frac{r_P^2-1}{12r_P} + \sum_{j=1}^{i_{P,t}-1}\frac{\overline{b_P j}(r_P-\overline{b_P j})}{2r_P}.$$

If $q > 2$, then $\chi(-A) = 0$. Using this equality we obtain (see [Suz04])

$$A^3 = \frac{12}{(q-1)(q-2)}\left(1 - \frac{A\cdot c_2}{12} + \sum_{P\in B} c_P(-A)\right). \tag{2.5}$$

In the above notation, applying (2.2), Serre duality and Kawamata-Viehweg vanishing to $D = K_X$, we get the following important equality (see, e.g., [Rei87]):

$$24 = -K_X\cdot c_2(X) + \sum_{P\in\mathbf{B}}\left(r_P - \frac{1}{r_P}\right). \tag{2.6}$$

Theorem 2.7 ([Kaw92a], [KMMT00]). *In the above notation,*

$$-K_X\cdot c_2(X) \ge 0, \qquad \sum_{P\in\mathbf{B}}\left(r_P - \frac{1}{r_P}\right) \le 24. \tag{2.8}$$

Proposition 2.9. *Let X be a Fano threefold with terminal singularities and let Ξ be an n-torsion element in the Weil divisor class group. Let $\mathbf{B}^{\Xi}$ be the collection of points $P \in \mathbf{B}$ where Ξ is not Cartier. Then*

$$2 = \sum_{P\in\mathbf{B}^{\Xi}}\frac{\overline{b_P i_{\Xi,P}}\ \left(r_P - \overline{b_P i_{\Xi,P}}\right)}{2r_P}. \tag{2.10}$$

where $i_{\Xi,P}$ *is taken so that* $\Xi \sim i_{\Xi,P} K_X$ *near* $P \in \mathbf{B}$ *and* $\overline{}$ *is the residue* mod r_P. *Assume furthermore that* n *is prime. Then*

(i) $n \in \{2, 3, 5, 7\}$.
(ii) *If* $n = 7$, *then* $\mathbf{B}^{\Xi} = (7, 7, 7)$.[†]
(iii) *If* $n = 5$, *then* $\mathbf{B}^{\Xi} = (5, 5, 5, 5)$, $(10, 5, 5)$, *or* $(10, 10)$.
(iv) *If* $n = 3$, *then* $\sum_{P \in \mathbf{B}^{\Xi}} r_P = 18$.
(v) *If* $n = 2$, *then* $\sum_{P \in \mathbf{B}^{\Xi}} r_P = 16$.

Proof. By Kawamata-Viehweg vanishing theorem, Riemann-Roch (2.2), and Serre duality we have $\chi(\mathscr{O}_X) = 1$,

$$0 = \chi(\Xi) = 1 + \textstyle\sum_P c_P(\Xi),$$

$$0 = \chi(K_X + \Xi) = 1 + \tfrac{1}{12} K_X \cdot c_2(X) + \textstyle\sum_{P \in \mathbf{B}} c_P(K_X + \Xi).$$

Subtracting we get

$$0 = -\frac{1}{12} K_X \cdot c_2(X) + \sum_{P \in \mathbf{B}} (c_P(\Xi) - c_P(K_X + \Xi)).$$

Since $n i_{\Xi,P} \equiv 0 \mod r_P$,

$$0 = -\frac{1}{12} K_X \cdot c_2(X) + \frac{1}{12} \sum_{P \in \mathbf{B}} \left(r_P - \frac{1}{r_P} \right) - \sum_{P \in \mathbf{B}} \frac{\overline{b_P i_{\Xi,P}} \; \left(r_P - \overline{b_P i_{\Xi,P}} \right)}{2 r_P}.$$

This proves (2.10).
Now assume that n is prime. If $P \in \mathbf{B}^{\Xi}$, then $n \mid r_P$. Write $r_P = n r'_P$. Since $r_P \mid n i_P$, $i_P = r'_P i'_P$, where $n \nmid i'_P$. Let $\overline{(\quad)}_n$ be the residue mod n. Then

$$2 = \sum_{P \in \mathbf{B}^{\Xi}} \frac{\overline{b_P i'_{\Xi,P} r'} \; \left(n r'_P - \overline{b_P i'_{\Xi,P} r'_P} \right)}{2 n r'_P} = \frac{r'_P \overline{(b_P i'_{\Xi,P})_n} \; \left(n - \overline{(b_P i'_{\Xi,P})_n} \right)}{2n}.$$

Therefore,

$$4n^2 = \sum_{P \in \mathbf{B}^{\Xi}} r_P \overline{(b_P i'_{\Xi,P})_n} \; \left(n - \overline{(b_P i'_{\Xi,P})_n} \right).$$

Denote $\xi_P := \overline{(b_P i'_{\Xi,P})_n}$. Then $0 < \xi_P < n$, $\gcd(n, \xi_P) = 1$, and

$$4n = \sum_{P \in \mathbf{B}^{\Xi}} r'_P \xi_P \left(n - \xi_P \right) \geq \frac{n^2}{4} \sum_{P \in \mathbf{B}^{\Xi}} r'_P, \qquad 16 \geq n \sum_{P \in \mathbf{B}^{\Xi}} r'_P.$$

If $n \geq 11$, then $\sum r'_P = 1$, $n \mid r'_P$, and $r_P \geq n^2 \geq 121$, a contradiction. Therefore, $n \leq 7$. Consider the case $n = 7$. Then $\xi_P \left(n - \xi_P \right) = 6$, 10, or 12. The only solution is $\mathbf{B}^{\Xi} = (7, 7, 7)$. The case $n = 5$ is considered similarly. If $n = 3$, then $\xi_P \left(n - \xi_P \right) = 3$ and $\sum r_P = 3 \sum r'_P = 18$. Similarly, if $n = 2$, then $\xi_P \left(n - \xi_P \right) = 1$ and $\sum r_P = 2 \sum r'_P = 16$. This finishes the proof. □

[†]More delicate computations show that this case does not occur. (We do not need this.)

3. Computations with Riemann-Roch on $\mathbb{Q}$-Fano threefolds of large Fano index

Lemma 3.1 (see [Suz04]). *Let X be a Fano threefold with terminal singularities with $q := \mathrm{qW}(X)$, let $A := -\frac{1}{q}K_X$, and let r be the Gorenstein index of X. Then*

(i) *r and q are coprime;*
(ii) *rA^3 is an integer.*

Lemma 3.2. *Let X be a Fano threefold with terminal singularities.*

(i) *If $-K_X \sim qL$ for some Weil divisor L, then q divides $\mathrm{qW}(X)$.*
(ii) *If $-K_X \sim_{\mathbb{Q}} qL$ for some Weil divisor L, then q divides $\mathrm{q}\mathbb{Q}(X)$.*
(iii) *$\mathrm{qW}(X)$ divides $\mathrm{q}\mathbb{Q}(X)$.*
(iv) *Let $q := \mathrm{q}\mathbb{Q}(X)$ and let $K_X + qA \sim_{\mathbb{Q}} 0$. If the order of $K_X + qA$ in the group $\mathrm{Cl}(X)$ is prime to q, then $\mathrm{qW}(X) = \mathrm{q}\mathbb{Q}(X)$.*

Proof. To prove (i) write $-K_X \sim \mathrm{qW}(X)A$ and let $d = \gcd(\mathrm{qW}(X), q)$. Then $d = u\,\mathrm{qW}(X) + vq$ for some $u, v \in \mathbb{Z}$. Hence, $dA = u\,\mathrm{qW}(X)A + vqA \sim quL + qvA = q(uL + vA)$. Since A is a primitive element of $\mathrm{Cl}(X)$, $q = d$ and $q \mid \mathrm{qW}(X)$.
(ii) can proved similarly and (iii) is a consequence of (ii).
To show (iv) assume that $\Xi := K_X + qA$ is of order n. By our condition $qu + nv = 1$, where $u, v \in \mathbb{Z}$. Put $A' := A - u\Xi$. Then $qA' = qA - qu\Xi = qA - \Xi \sim -K_X$. Hence, $q = \mathrm{qW}(X)$ by (i) and (iii). □

Lemma 3.3. *Let X be a Fano threefold with terminal singularities.*

(i) *$\mathrm{q}\mathbb{Q}(X) \in \{1, \dots, 11, 13, 17, 19\}$.*
(ii) *If $\mathrm{q}\mathbb{Q}(X) \geq 5$, then $-K_X^3 \leq 125/2$.*

Proof. Denote $q := \mathrm{q}\mathbb{Q}(X)$ and write, as usual, $-K_X \sim_{\mathbb{Q}} qA$. Thus $n(K_X + qA) \sim 0$ for some positive integer n. The element $K_X + qA$ defines a cyclic étale in codimension one cover $\pi\colon X' \to X$ so that X' is a Fano threefold with terminal singularities and $K_{X'} + qA' \sim 0$, where $A' := \pi^*A$. Let $\sigma\colon X'' \to X'$ be a $\mathbb{Q}$-factorialization. (If X' is $\mathbb{Q}$-factorial, we take $X'' = X'$). Run K-MMP on X'': $\psi\colon X'' \dashrightarrow \bar{X}$. At the end we get a Mori-Fano fiber space $\bar{X} \to Z$. Let $A'' := \sigma^{-1}(A')$ and $\bar{A} := \psi_* A''$. Then $-K_{\bar{X}} \sim q\bar{A}$. If $\dim Z > 0$, then for a general fiber F of $\bar{X}/Z$, we have $-K_F \sim q\bar{A}|_F$. This is impossible because $q > 3$. Thus $\dim Z = 0$ and $\bar{X}$ is a $\mathbb{Q}$-Fano.
(i) By Lemma 3.2 the number q divides $\mathrm{qW}(\bar{X})$. On the other hand, by Theorem 1.1 we have $\mathrm{qW}(\bar{X}) \in \{1, \dots, 11, 13, 17, 19\}$. This proves (i).
To show (ii) we note that $-K_{\bar{X}}^3 \geq -K_{X''}^3 = -K_{X'}^3 \geq -K_{X''}^3$. Here the first inequality holds because for Fanos (with at worst log terminal singularities) the number $-\frac{1}{6}K^3$ is nothing but the leading term in the asymptotic Riemann-Roch and $\dim|-tK_{X''}| \leq \dim|-tK_{\bar{X}}|$. Now the assertion of (ii) follows from Theorem 1.2. □

From Lemmas 3.2 and 3.3 we have

Corollary 3.4. *Let X be a Fano threefold with terminal singularities.*

(i) *If $-K_X \sim qL$ for some Weil divisor L and $q \geq 5$, then $q = \mathrm{qW}(X)$.*
(ii) *If $-K_X \sim_{\mathbb{Q}} qL$ for some Weil divisor L and $q \geq 5$, then $q = \mathrm{q}\mathbb{Q}(X)$.*

Lemma 3.5 (cf. [Suz04]). *Let X be a Fano threefold with terminal singularities and let $q := \mathrm{qW}(X)$. Assume that $\mathrm{qW}(X) \geq 8$. Then one of the following holds:*

$q = 8$, $\mathbf{B} = (3^2, 5)$, $(3^2, 5, 9)$, $(3, 5, 11)$, $(3, 7)$, $(3, 9)$, $(5, 7)$, $(7, 11)$, $(7, 13)$, (11),
$q = 9$, $\mathbf{B} = (2, 4, 5)$, $(2^3, 5, 7)$, $(2, 5, 13)$,
$q = 10$, $\mathbf{B} = (7, 11)$,
$q = 11$, $\mathbf{B} = (2, 3, 5)$, $(2, 5, 7)$, $(2^2, 3, 4, 7)$,
$q = 13$, $\mathbf{B} = (3, 4, 5)$, $(2, 3^2, 5, 7)$,
$q = 17$, $\mathbf{B} = (2, 3, 5, 7)$,
$q = 19$, $\mathbf{B} = (3, 4, 5, 7)$.

In all cases the group $\mathrm{Cl}(X)$ is torsion free.

Proof. We use a computer program written in PARI [PARI] ‡. Below is the description of our algorithm.
Step 1. By Theorem 2.7 we have $\sum_{P\in\mathbf{B}}(1 - 1/r_P) \leq 24$. Hence there is only a finite (but very huge) number of possibilities for the basket $\mathbf{B} = \{[r_P, b_P]\}$. In each case we know $-K_X \cdot c_2(X)$ from (2.6). Let $r := \mathrm{lcm}(\{r_P\})$ be the Gorenstein index of X.
Step 2. By Lemma 3.3 $\mathrm{q}\mathbb{Q}(X) \in \{8, \dots, 11, 13, 17, 19\}$. Moreover, the condition $\gcd(q, r) = 1$ (see Lemma 3.1) eliminates some possibilities.
Step 3. In each case we compute A^3 and $-K_X^3 = q^3A^3$ by formula (2.5). Here, for $D = -A$, the number i_P is uniquely determined by $qi_P \equiv b_P \mod r_P$ and $0 \leq i_P < r_P$. Further, we check the condition $rA^3 \in \mathbb{Z}$ (Lemma 3.1) and the inequality $-K_X^3 \leq 125/2$ (Lemma 3.3).
Step 4. Finally, by the Kawamata-Viehweg vanishing theorem we have $\chi(tA) = h^0(tA)$ for $-q < t$. We compute $\chi(tA)$ by using (2.4) and check conditions $\chi(tA) = 0$ for $-q < t < 0$ and $\chi(tA) \geq 0$ for $t > 0$.
At the end we get our list. To prove the last assertion assume that $\mathrm{Cl}(X)$ contains an n-torsion element Ξ. Clearly, we also may assume that n is prime. By Proposition 2.9 we have $\sum_{n|r_i} r_i \geq 16$. Moreover, $\sum_{n|r_i} r_i \geq 18$ if $n = 3$. This does not hold in any case of our list. □

Proposition 3.6. *Let X be a $\mathbb{Q}$-Fano threefold with $\mathrm{q}\mathbb{Q}(X) \geq 9$. Let $q := \mathrm{q}\mathbb{Q}(X)$ and let $-K_X \sim_{\mathbb{Q}} qA$. Then the group $\mathrm{Cl}(X)$ is torsion free, $\mathrm{qW}(X) = \mathrm{q}\mathbb{Q}(X)$, and one of the following holds:*

‡The PARI code is available at `http://mech.math.msu.su/department/algebra/staff/prokhorov/q-fano`.

q	$\mathbf{B}$	A^3	$\dim\lvert kA\rvert$							
			$\lvert A\rvert$	$\lvert 2A\rvert$	$\lvert 3A\rvert$	$\lvert 4A\rvert$	$\lvert 5A\rvert$	$\lvert 6A\rvert$	$\lvert 7A\rvert$	$\lvert -K\rvert$
9	$(2,4,5)$	$\frac{1}{20}$	0	1	2	4	6	8	11	19
9	$(2,2,2,5,7)$	$\frac{1}{70}$	-1	0	0	1	1	2	3	5
10	$(7,11)$	$\frac{2}{77}$	-1	0	1	1	3	4	6	13
11	$(2,3,5)$	$\frac{1}{30}$	0	1	2	3	5	7	9	23
11	$(2,5,7)$	$\frac{1}{70}$	0	0	0	1	2	3	4	10
11	$(2,2,3,4,7)$	$\frac{1}{84}$	-1	0	0	1	1	2	3	8
13	$(3,4,5)$	$\frac{1}{60}$	0	0	1	2	3	4	5	19
13	$(2,3,3,5,7)$	$\frac{1}{210}$	-1	-1	0	0	0	1	1	5
17	$(2,3,5,7)$	$\frac{1}{210}$	-1	0	0	0	1	1	2	12
19	$(3,4,5,7)$	$\frac{1}{420}$	-1	-1	0	0	0	0	1	8

Proof. First we claim that $\mathrm{qW}(X) = \mathrm{q}\mathbb{Q}(X)$. Assume the converse. Then, as in the proof of Lemma 3.3, the class of $K_X + qA$ is a non-trivial n-torsion element in $\mathrm{Cl}(X)$ defining a global cover $\pi\colon X' \to X$. We have $K_{X'} + qA' \sim 0$, where $A' = \pi^*A$. Hence X' is such as in Lemma 3.5 and by Corollary 3.5 we have $\mathrm{Cl}(X') \simeq \mathbb{Z}\cdot A'$ and $\mathrm{qW}(X') = \mathrm{q}\mathbb{Q}(X') \ge q$. The Galois group $\boldsymbol{\mu}_n$ acts naturally on X'. Consider, for example, the case $q = 11$ and $\mathbf{B}_{X'} = (2, 3, 5)$ (all other cases are similar). Then X' has three cyclic quotient singularities whose indices are 2, 3, and 5. These points must be $\boldsymbol{\mu}_n$-invariant. Hence the variety X has cyclic quotient singularities of indices $2n$, $3n$, and $5n$. By Lemma 3.2 we have $\gcd(q, n) \ne 1$. In particular, $n \ge 11$. This contradicts (2.8). Therefore, $\mathrm{qW}(X) = \mathrm{q}\mathbb{Q}(X)$ and so X is such as in Lemma 3.5.
Now we have to exclude only the case $q = 9$, $\mathbf{B} = (2, 5, 13)$. But in this case by (2.6) and (2.5) we have $A^3 = 9/130$ and $-K_X \cdot c_2 = 621/130$. On the other hand, by Kawamata-Bogomolov's bounds [Kaw92a] we have $2673/130 = (4q^2 - 3q)A^3 \le 4K_X \cdot c_2 = 1242/65$ [Suz04, Proposition 2.2]. The contradiction shows that this case is impossible. Finally, the values of A^3 and dimensions of $|kA|$ are computed by using (2.5) and (2.4). □

Corollary 3.7. *Let X be a $\mathbb{Q}$-Fano threefold satisfying assumptions of* (i)-(v) *of Theorem* 1.4. *Then X has only cyclic quotient singularities.*

Proof. Indeed, in these cases the indices of points in the basket $\mathbf{B}$ are distinct numbers and moreover $\mathbf{B}$ contains no pairs of points of indices 2 and 4. Then the assertion follows by [Mor85a], or [Rei87] □

Corollary 3.8. *Let X be a $\mathbb{Q}$-Fano threefold with* $\mathrm{q}\mathbb{Q}(X) \ge 9$. *Then* $\dim|A| \le 0$.

Computer computations similar to that in Lemma 3.5 allow us to prove the following.

Lemma 3.9. *Let X be a Fano threefold with terminal singularities, let $q := \mathrm{qW}(X)$, and let $A := -\frac{1}{q}K_X$.*

(i) *If $q \geq 5$ and $\dim|A| > 1$, then $q = 5$, $\mathbf{B} = (2)$, and $A^3 = 1/2$.*
(ii) *If $q \geq 7$ and $\dim|A| > 0$, then $q = 7$, $\mathbf{B} = (2, 3)$, $A^3 = 1/6$.*

3.10. Proof of (vi) and (vii) of Theorem 1.4. (vii) Apply Lemma 3.9. Then the result is well-known: in fact, $2A$ is Cartier and by Riemann-Roch $\dim|2A| = 6 = \dim X + 3$. Hence X is a variety of Δ-genus zero [Fuj75], i.e., a variety of minimal degree. Then $X \simeq \mathbb{P}(1^3, 2)$.
(vi) Put $q := \mathrm{q}\mathbb{Q}(X)$, $\Xi := K_X + qA$, and $\Xi_1 := A - A_1$. By our assumption $n\Xi \sim n\Xi_1 \sim 0$ for some integer n. If either $\Xi \not\sim 0$ or $\Xi_1 \not\sim 0$, then elements Ξ and Ξ' define an étale in codimension one finite cover $\pi\colon X' \to X$ such that $K_{X'} + qA' \sim 0$ and $A' \sim A_1'$, where $A' := \pi^*A$ and $A_1' := \pi^*A_1$. If $\Xi \sim \Xi_1 \sim 0$, we put $X' = X$. In both cases, the following inequalities hold: $\mathrm{qW}(X') \geq 7$ and $\dim|A'| \geq 1$. By Lemma 3.9 we have $\mathbf{B}(X') = (2, 3)$ and $\mathrm{q}\mathbb{Q}(X') = \mathrm{qW}(X') = 7$. Note that the Gorenstein index of X' is strictly less than $\mathrm{qW}(X')$. In this case, $X' \simeq \mathbb{P}(1^2, 2, 3)$ according to [San96]. [§] Now it is sufficient to show that π is an isomorphism. Assume the converse. By our construction, there is an action of a cyclic group $\boldsymbol{\mu}_p \subset \mathrm{Gal}(X'/X)$, p is prime, such that π is decomposed as $\pi\colon X' \to X'/\boldsymbol{\mu}_p \to X$. Here $X'/\boldsymbol{\mu}_p$ is a $\mathbb{Q}$-Fano threefold and there is a torsion element of $\mathrm{Cl}(X'/\boldsymbol{\mu}_p)$ which is not Cartier exactly at points where $X' \to X'/\boldsymbol{\mu}_p$ is not étale. There are exactly four such points and two of them are points of indices 2 and 3. Thus the basket of $X'/\boldsymbol{\mu}_p$ consists of points of indices p, p, $2p$, and $3p$. This contradicts Proposition 2.9.

Lemma 3.11. *Let X be a $\mathbb{Q}$-Fano threefold with $q := \mathrm{q}\mathbb{Q}(X)$. If there are three effective different Weil divisors A, A_1, A_2 such that $-K_X \sim_{\mathbb{Q}} qA \sim_{\mathbb{Q}} qA_1 \sim_{\mathbb{Q}} qA_2$ and $A \not\sim A_1$, then $q \leq 5$.*

Proof. Assume that $q \geq 6$. As in 3.10 consider a cover $\pi\colon X' \to X$. Thus on X' we have $A' \sim A_1' \sim A_2'$ and $-K_{X'} \sim qA'$. Moreover, $\dim|A'| = 1$ according to Lemma 3.9. In this case, the action of $\mathrm{Gal}(X'/X)$ on the pencil $|A'|$ is trivial (because there are three invariant members A', A_1', and A_2'). But then $A \sim A_1 \sim A_2$, a contradiction. □

4. Birational construction

4.1. Let X be a $\mathbb{Q}$-Fano threefold and let A be the ample Weil divisor that generates the group $\mathrm{Cl}(X)/\sim_{\mathbb{Q}}$. Thus we have $-K_X \sim_{\mathbb{Q}} qA$. Let $\mathscr{M}$ be a mobile linear system without fixed components and let $c := \mathrm{ct}(X, \mathscr{M})$ be the canonical threshold of $(X, \mathscr{M})$. So the pair $(X, c\mathscr{M})$ is canonical but not terminal. Assume that $-(K_X + c\mathscr{M})$ is ample.

Recall that, for any point $P \in X$, the class of K_X is a generator of the local Weil divisor class group $\mathrm{Cl}(X, P)$.

[§] The result also can be easily proved by using birational transformations similar to that in §4.

Lemma 4.2. *Let $P \in X$ be a point of index $r > 1$. Assume that $\mathscr{M} \sim -mK_X$ near P, where $0 < m < r$. Then $c \le 1/m$.*

Proof. According to [Kaw92b] there is an exceptional divisor Γ over P of discrepancy $a(\Gamma) = 1/r$. Let $\varphi\colon Y \to X$ be a resolution. Clearly, Γ is a prime divisor on Y. Write

$$K_Y = \varphi^* K_X + \frac{1}{r}\Gamma + \sum \delta_i \Gamma_i, \quad \mathscr{M}_Y = \varphi^*\mathscr{M} - \operatorname{ord}_\Gamma(\mathscr{M})\Gamma - \operatorname{ord}_{\Gamma_i}(\mathscr{M})\Gamma_i,$$

where $\mathscr{M}_Y$ is the birational transform of $\mathscr{M}$ and Γ_i are other φ-exceptional divisors. Then

$$K_Y + c\mathscr{M}_Y = \varphi^*(K_X + c\mathscr{M}) + (1/r - c\operatorname{ord}_\Gamma(\mathscr{M}))\Gamma + \dots$$

and so $1/r - c\operatorname{ord}_\Gamma(\mathscr{M}) \ge 0$. On the other hand, $\operatorname{ord}_\Gamma(\mathscr{M}) \equiv m/r \mod \mathbb{Z}$ (because $mK_X + \mathscr{M} \sim 0$ near P). Hence, $\operatorname{ord}_\Gamma(\mathscr{M}) \ge m/r$ and $c \le 1/m$. □

4.3. In the construction below we follow [Ale94]. Let $f\colon \tilde{X} \to X$ be a $K + c\mathscr{M}$-crepant blowup such that $\tilde{X}$ has only terminal $\mathbb{Q}$-factorial singularities:

$$K_{\tilde{X}} + c\tilde{\mathscr{M}} = f^*(K_X + c\mathscr{M}). \tag{4.4}$$

As in [Ale94], we run $K + c\mathscr{M}$-MMP on $\tilde{X}$. We get the following diagram (Sarkisov link of type I or II)

$$\begin{array}{ccccc} & \tilde{X} & \dashrightarrow & \bar{X} & \\ {}^{f}\swarrow & & & & \searrow^{g} \\ X & & & & \hat{X} \end{array} \tag{4.5}$$

where the varieties $\tilde{X}$ and $\bar{X}$ have only $\mathbb{Q}$-factorial terminal singularities, $\rho(\tilde{X}) = \rho(\bar{X}) = 2$, f is a Mori extremal divisorial contraction, $\tilde{X} \dashrightarrow \bar{X}$ is a sequence of log flips, and g is a Mori extremal contraction (either divisorial or fiber type). Thus one of the following possibilities holds:

a) $\dim \hat{X} = 1$ and g is a $\mathbb{Q}$-del Pezzo fibration;
b) $\dim \hat{X} = 2$ and g is a $\mathbb{Q}$-conic bundle; or
c) $\dim \hat{X} = 3$, g is a divisorial contraction, and $\hat{X}$ is a $\mathbb{Q}$-Fano threefold. In this case, denote $\hat{q} := \mathrm{q}\mathbb{Q}(\hat{X})$.

Let E be the f-exceptional divisor. In all what follows, for a divisor D on X, let $\tilde{D}$ and $\bar{D}$ denote strict birational transforms of D on $\tilde{X}$ and $\bar{X}$, respectively. If g is birational, we put $\hat{D} := g_*\bar{D}$.

Claim 4.6 ([Ale94]). *If the map g of (4.5) is birational, then $\bar{E}$ is not an exceptional divisor. If g is of fiber type, then $\bar{E}$ is not composed of fibers.*

Proof. Assume the converse. If g is birational, this implies that the map $g \circ \chi \circ f^{-1}\colon X \dashrightarrow \hat{X}$ is an isomorphism in codimension 1. Since both X and $\hat{X}$ are Fano threefolds, this implies that $g \circ \chi \circ f^{-1}$ is in fact an isomorphism. On the other hand, the number of $K + c\mathscr{M}$-crepant divisors on $\hat{X}$ is less than that on X, a contradiction. If $\dim \hat{X} \le 2$, then $\bar{E}$ is a pull-back of an ample

Weil divisor on $\hat{X}$. But then $n\bar{E}$ is a movable divisor for some $n > 0$. This contradicts exceptionality of E. □

4.7. Notation. If $|kA| \neq \varnothing$, let $S_k \in |kA|$ be a general member. Write

$$
\begin{aligned}
K_{\tilde{X}} &= f^*K_X + \alpha E,\\
\tilde{S}_k &= f^*S_k - \beta_k E, \qquad (4.8)\\
\tilde{\mathscr{M}} &= f^*\mathscr{M} - \beta_0 E.
\end{aligned}
$$

Then

$$c = \alpha/\beta_0. \qquad (4.9)$$

Remark 4.10. If $\alpha < 1$, then $a(E, |-K_X|) < 1$. On the other hand, $0 = K_X + |-K_X|$ is Cartier. Hence, $a(E, |-K_X|) \leq 0$ and $K_{\tilde{X}} + f_*^{-1}|-K_X|$ is linearly equivalent to a non-positive multiple of E. Therefore, $f_*^{-1}|-K_X| \subset |-K_{\tilde{X}}|$ and so

$$\dim|-K_{\bar{X}}| = \dim|-K_{\tilde{X}}| \geq \dim|-K_X|.$$

In our situation X has only cyclic quotient singularities (see Corollary 3.7). So, the following result is very important.

Theorem 4.11 ([Kaw96]). *Let $(Y \ni P)$ be a terminal cyclic quotient singularity of type $\frac{1}{r}(1, a, r-a)$, let $f\colon \tilde{Y} \to Y$ be a Mori divisorial contraction, and let E be the exceptional divisor. Then $f(E) = P$, f is the weighted blowup with weights $(1, a, r-a)$ and the discrepancy of E is $a(E) = 1/r$.*

We call this f the *Kawamata blowup* of P.

4.12. Notation. Assume that g is birational. Let $\bar{F}$ be the g-exceptional divisor and let $\tilde{F}$ and F be its proper transforms on $\tilde{X}$ and X, respectively. Let n be the maximal integer dividing the class of $\bar{F}$ in $\mathrm{Cl}(\bar{X})$. Let Θ be an ample Weil divisor on $\hat{X}$ that generates $\mathrm{Cl}(\hat{X})/{\sim_{\mathbb{Q}}}$. Write

$$\hat{S}_k \sim_{\mathbb{Q}} s_k\Theta \quad \text{and} \quad \hat{E} \sim_{\mathbb{Q}} e\Theta,$$

where s_k, $e \in \mathbb{Z}$, $s_k \geq 0$, $e \geq 1$. Note that $s_k = 0$ if and only if $\bar{S}_k$ is contracted by g.

Lemma 4.13. *In the above notation assume that the group $\mathrm{Cl}(X)$ is torsion free. Write $F \sim dA$, where $d \in \mathbb{Z}$, $d \geq 1$. Then $\mathrm{Cl}(\hat{X}) \simeq \mathbb{Z} \oplus \mathbb{Z}_n$ and $d = ne$.*

Proof. Write $\bar{F} \sim n\bar{G}$, where $\bar{G}$ is an integral Weil divisor. Then $\bar{E} \sim e\bar{\Theta} + k\bar{G}$ for some $k \in \mathbb{Z}$ and $\mathrm{Cl}(\hat{X}) \simeq \mathrm{Cl}(\bar{X})/\bar{F}\mathbb{Z} \simeq \mathbb{Z} \oplus \mathbb{Z}_n$. We have

$$\mathbb{Z}_d \simeq \mathrm{Cl}(X)/\langle F\rangle \simeq \mathrm{Cl}(\bar{X})/\langle \bar{E}, \bar{F}\rangle \simeq \mathbb{Z} \oplus \mathbb{Z}/\langle e\bar{\Theta} + k\bar{G}, n\bar{G}\rangle.$$

Since the last group is of order ne, we have $d = ne$. □

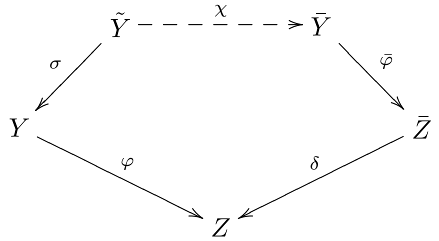
From now until the end of this section we consider the case where $\hat{X}$ is a surface.

Lemma 4.14. *Assume that $\hat{X}$ is a surface. Then $\hat{X}$ is a del Pezzo surface with Du Val singularities of type A_n. The linear system $|-K_{\hat{X}}|$ is base point free. If moreover the group $\mathrm{Cl}(X)$ is torsion free, then so is $\mathrm{Cl}(\hat{X})$ and there are only the following possibilities:*

(i) $K_{\hat{X}}^2 = 9$, $\hat{X} \simeq \mathbb{P}^2$;
(ii) $K_{\hat{X}}^2 = 8$, $\hat{X} \simeq \mathbb{P}(1^2, 2)$;
(iii) $K_{\hat{X}}^2 = 6$, $\hat{X} \simeq \mathbb{P}(1, 2, 3)$;
(iv) $K_{\hat{X}}^2 = 5$, *$\hat{X}$ has a unique singular point, point of type A_4.*

Proof. By the main result of [MP08b] the surface $\hat{X}$ has only Du Val singularities of type A_n. Since $\rho(\hat{X}) = 1$ and $\hat{X}$ is uniruled, $-K_{\hat{X}}$ is ample. Further, since both $\bar{X}$ and $\hat{X}$ have only isolated singularities and $\mathrm{Pic}(\bar{X}/\hat{X}) \simeq \mathbb{Z}$, there is a well-defined injective map $g^*\colon \mathrm{Cl}(\hat{X}) \to \mathrm{Cl}(\bar{X})$. Hence the group $\mathrm{Cl}(\hat{X})$ is torsion free whenever $\mathrm{Cl}(X)$ is. The remaining part follows from the classification of del Pezzo surfaces with Du Val singularities (see, e.g., [MZ88]). □

Lemma 4.15. *Let $\varphi\colon Y \to Z$ be a $\mathbb{Q}$-conic bundle (we assume that Y is $\mathbb{Q}$-factorial and $\rho(Y/Z) = 1$). Suppose that there are two prime divisors D_1 and D_2 such that $\varphi(D_i) = Z$, the log divisor $K_Y + D_1 + D_2$ is φ-linearly trivial and canonical. Suppose furthermore that Z is singular and let $o \in Z$ be a singular point. Then $o \in Z$ is of type A_{r-1} for some $r \geq 2$ and there is a Sarkisov link*



where σ is the Kawamata blowup of a cyclic quotient singularity $\frac{1}{r}(1, a, r-a)$ over o, χ is a sequence of flips, $\bar{\varphi}$ is a $\mathbb{Q}$-conic bundle with $\rho(\bar{Y}/\bar{Z}) = 1$, and δ is a crepant contraction of an irreducible curve to o. Moreover, if $\bar{D}_i$ is the proper transform of D_i on $\bar{Y}$, then the divisor $K_{\bar{Y}} + \bar{D}_1 + \bar{D}_2$ is linearly trivial over Z and canonical.

Proof. Regard Y/Z as an algebraic germ over o. Since D_i are generically sections, the fibration φ has no discriminant curve. By [MP08c] the central fiber $C := \varphi^{-1}(o)_{\mathrm{red}}$ is irreducible and by the main result of [MP08b] Y/Z is toroidal, that is, it is analytically isomorphic to a toric contraction:

$$Y \simeq (\mathbb{C}^2 \times \mathbb{P}^1)/\boldsymbol{\mu}_r(a, r-a, 1)$$

for some r, $a \in \mathbb{Z}$ with $r \geq 2$ and $\gcd(a, r) = 1$. Here the map $Y \to Z$ is the projection to $Z \simeq \mathbb{C}^2/\boldsymbol{\mu}_r(a, r-a)$. In particular, Y has exactly two singular points and these points are cyclic quotients of types $\frac{1}{r}(1, a, r-a)$ and

$\frac{1}{r}(-1,a,r-a)$. Since the pair (Y, D_1+D_2) is canonical, $D_1 \cap D_2 = \varnothing$. On the other hand, the divisor $D_1+D_2 \sim -K_Y$ must contain all points on indices >1. Hence $\operatorname{Sing}(Y) = (D_1+D_2)\cap C$. Further, the divisors D_i are quotients of two disjointed sections of $\mathbb{C}^2 \times \mathbb{P}^1 \to \mathbb{C}^2$ by $\boldsymbol{\mu}_r$. Therefore, $D_i \cdot C = 1/r$. Now consider the Kawamata blowup $\sigma : \tilde{Y} \to Y$ of $C \cap D_1$. Let E be the exceptional divisor and let $\tilde{D}_i$ be the proper transform of D_i. Since $K_{\tilde{Y}} = \sigma^* K_Y + \frac{1}{r}E$ and the pair (Y, D_1+D_2) is canonical, we have

$$K_{\tilde{Y}} + \tilde{D}_1 + \tilde{D}_2 = \sigma^*(K_Y + D_1 + D_2).$$

It is easy to check locally that the proper transform $\tilde{C}$ of the central fiber C does not meet $\tilde{D}_1$. Moreover, $\tilde{C}\cap E$ is a smooth point of $\tilde{Y}$ and E. Thus we have $\tilde{D}_1 \cdot \tilde{C} = 0$, $E\cdot \tilde{C} = 1$, and $\tilde{D}_2 \cdot \tilde{C} = D_2 \cdot C = 1/r$. Hence, $K_{\tilde{Y}} \cdot \tilde{C} = -1/r$. Since the set-theoretical fiber over o in $\tilde{Y}$ coincides with $E \cup \tilde{C}$, the divisor $-K_{\tilde{Y}}$ is ample over Z and $\tilde{C}$ generates a (flipping) extremal ray R. Run the MMP over Z in this direction, i.e., starting with R. Assume that we end up with a divisorial contraction $\bar{\varphi}\colon \bar{Y} \to \bar{Z}$. Then $\bar{\varphi}$ must contract the proper transform $\bar{E}$ of E. Here $\bar{Z}/Z$ is a Mori conic bundle and the map $Y \dashrightarrow \bar{Z}$ is an isomorphism in codimension one, so it is an isomorphism. Moreover, $\bar{Z}/Z$ has a section, the proper transforms of D_i. Hence the fibration $\bar{Z}/Z$ is toroidal over o. Consider Shokurov's difficulty [Sho85]

$$\mathrm{d}(W) := \#\{\text{exceptional divisors of discrepancy} < 1\}.$$

Then $\mathrm{d}(Y) = \mathrm{d}(\bar{Z}) = 2(r-1)$. On the other hand,

$$\mathrm{d}(\bar{Z}) - 1 \le \mathrm{d}(\bar{Y}) < \mathrm{d}(\tilde{Y}) = r-1+a-1+r-a-1 = 2r-3$$

(because the map $\tilde{Y} \dashrightarrow \bar{Y}$ is not an isomorphism). The contradiction shows that our MMP ends up with a $\mathbb{Q}$-conic bundle. Clearly, the divisor $K_{\bar{Y}}+\bar{D}_1+\bar{D}_2$ is linearly trivial and canonical. By [MP08b] the surface $\bar{Z}$ has at worst Du Val singularities of type A. Hence the morphism δ is crepant [Mor85b]. □

Corollary 4.16. *In the above notation assume that* $\bar{Y}$ *is a toric variety. Then so is* Y.

Corollary 4.17. *Notation as in Lemma* 4.15. *Assume that the base surface* Z *is toric. Then so is* Y.

Proof. Induction by the number e of crepant divisors of Z. If $e = 0$, then Y is smooth and $Y \simeq \mathbb{P}(\mathscr{E})$, where $\mathscr{E}$ is a decomposable rank-2 vector bundle on Z. □

Proposition 4.18. *In notation of* 4.3, *let* $\hat{X}$ *be a surface. Let* $\Gamma \in |-K_{\hat{X}}|$ *and let* $G := g^{-1}(\Gamma)$. *Suppose that there are two prime divisors* D_1 *and* D_2 *such that* $g(D_i) = \hat{X}$ *and* $K_{\hat{X}} + D_1 + D_2 + G \sim 0$. *Then the pair* $(\bar{X}, D_1 + D_2)$ *is canonical. If furthermore the surface* $\hat{X}$ *is toric, then so are* $\bar{X}$ *and* X.

Proof. Clearly, we may replace Γ with a general member of $|-K_{\hat{X}}|$. Note that G is an elliptic ruled surface and $K_G + D_1|_G + D_2|_G \sim 0$. Hence divisors

$D_1|_G$ and $D_2|_G$ are disjointed sections. This shows that $D_1 \cap D_2$ is either empty or consists of fibers. Assume that $D_1 \cap D_2 \neq \varnothing$. We can take Γ so that $G \cap D_1 \cap D_2 = \varnothing$. By adjunction $-K_{D_1} \sim \bar{G}|_{D_1} + D_2|_{D_1}$. Since D_1 is a rational surface (birational to $\hat{X}$), the divisor $\bar{G}|_{D_1} + D_2|_{D_1}$ must be connected, a contradiction. Thus, $D_1 \cap D_2 = \varnothing$.
Therefore both divisors D_1 and D_2 contain no fibers and so $D_1 \simeq D_2 \simeq \hat{X}$. Then the pair $(\bar{X}, D_1 + D_2)$ is PLT by the Inversion of Adjunction. Since $K_{\bar{X}} + D_1 + D_2$ is Cartier, this pair must be canonical. The second assertion follows by Corollary 4.17. □

5. Case $\mathrm{q}\mathbb{Q}(X) = 10$

Consider the case $\mathrm{q}\mathbb{Q}(X) = 10$. We assume that a $\mathbb{Q}$-Fano threefold with $\mathrm{q}\mathbb{Q}(X) = 10$ exists and get a contradiction applying Construction (4.5).
By Proposition 3.6 the group $\mathrm{Cl}(X)$ is torsion free and $\mathbf{B} = (7, 11)$. Recall also that

$$|A| = \varnothing, \quad \dim|2A| = 0, \quad \text{and} \quad \dim|3A| = 1. \tag{5.1}$$

For $r = 7$ and 11, let P_r be a (unique) point of index r. In notation of §4, take $\mathscr{M} := |3A|$. By (5.1) there exist a (unique) irreducible divisor $S_2 \in |-2K_X|$ and $\mathscr{M}$ is a pencil without fixed components. Let $S_3 \in \mathscr{M} = |3A|$ be a general member.
Apply Construction (4.5). Notations of 4.3 and 4.7 will be used freely. Near P_{11} we have $A \sim -10K_X$, so $\mathscr{M} \sim -8K_X$. By Lemma 4.2 we get $c \leq 1/8$. In particular, the pair $(X, \mathscr{M})$ is not canonical. For some a_1, $a_2 \in \mathbb{Z}$ we can write

$$\begin{aligned} K_{\tilde{X}} + 5\tilde{S}_2 &= f^*(K_X + 5S_2) - a_1E &&\sim -a_1E, \\ K_{\tilde{X}} + 2\tilde{S}_2 + 2\tilde{S}_3 &= f^*(K_X + 2S_2 + 2S_3) - a_2E &&\sim -a_2E. \end{aligned}$$

Therefore,

$$\begin{aligned} K_{\bar{X}} + 5\bar{S}_2 + a_1\bar{E} &\sim 0, \\ K_{\bar{X}} + 2\bar{S}_2 + 2\bar{S}_3 + a_2\bar{E} &\sim 0, \end{aligned} \tag{5.2}$$

where $\dim|S_2| = 0$ and $\dim|S_3| = 1$. Using (4.8) we obtain

$$\begin{aligned} 5\beta_2 &= a_1 + \alpha, \\ 2\beta_2 + 2\beta_3 &= a_2 + \alpha. \end{aligned} \tag{5.3}$$

Since $S_3 \in \mathscr{M}$ is a general member, by (4.9) we have $c = \alpha/\beta_3 \leq 1/8$, so

$$8\alpha \leq \beta_3 \quad \text{and} \quad a_2 \geq 15\alpha + 2\beta_2. \tag{5.4}$$

5.5. First we consider the case where $f(E)$ is either a curve or a Gorenstein point on X. Then α and β_k are non-negative integers. In particular, $a_2 \geq 15$. From (5.2) and (5.4) we obtain that g is birational. Indeed, otherwise restricting the second relation of (5.2) to a general fiber V we get that $-K_V$ is divisible by some number $a' \geq a_2 \geq 15$. This is impossible because V is either $\mathbb{P}^1$ or a smooth del Pezzo surface.

Thus g is birational and $\hat{X}$ is a $\mathbb{Q}$-Fano. Again from (5.2) and (5.4) in notation of 4.12 we get

$$-K_{\hat{X}} \sim 2\hat{S}_2 + 2\hat{S}_3 + a_2\hat{E} \sim_{\mathbb{Q}} (2s_2 + 2s_3 + a_2e)\Theta,$$

where $s_2,\ s_3 \geq 0$, $e \geq 1$, and $a_2 \geq 15$. This immediately gives us $\mathrm{q}\mathbb{Q}(\hat{X}) \geq 15$ and $e = 1$, that is, $\hat{E} \sim_{\mathbb{Q}} \Theta$. By Proposition 3.6 the group $\mathrm{Cl}(\hat{X})$ is torsion free. In particular, $\hat{E} \sim \Theta$ and $|\Theta| \neq \varnothing$. On the other hand, again by Proposition 3.6 we have $|\Theta| = \varnothing$, a contradiction.

5.6. Therefore $f(E)$ is a non-Gorenstein point P_r of index $r = 7$ or 11. By Theorem 4.11 f is Kawamata blowup and $\alpha = 1/r$. Near P_r we can write $A \sim -l_rK_X$, where $l_r \in \mathbb{Z}$ and $10l_r \equiv 1 \mod r$. Then $S_k + kl_rK_X$ is Cartier near P_r. Therefore, $\beta_k \equiv kl_r\alpha \mod \mathbb{Z}$ and so $\beta_k = kl_r/r + m_k$, where $m_k = m_{k,r} \in \mathbb{Z}$. Explicitly, we have the following values of α, β_k, and a_k:

r	α	β_2	β_3	a_1	a_2
7	$\frac{1}{7}$	$\frac{3}{7} + m_2$	$\frac{1}{7} + m_3$	$2 + 5m_2$	$1 + 2m_2 + 2m_3$
11	$\frac{1}{11}$	$\frac{9}{11} + m_2$	$\frac{8}{11} + m_3$	$4 + 5m_2$	$3 + 2m_2 + 2m_3$

Claim 5.7. *If $r = 7$, then $m_3 \geq 1$.*

Proof. Follows from $c = \alpha/\beta_3 \leq 1/8$. □

If g is not birational, then, as above, restricting relations (5.2) to a general fiber V we get

$$-K_V \sim 5\bar{S}_2|_V + a_1\bar{E}|_V \sim 2\bar{S}_2|_V + 2\bar{S}_3|_V + a_2\bar{E}|_V,$$

where $E|_V \neq 0$ and $S_2|_V$, $S_3|_V$, and $E|_V$ are proportional to $-K_V$ (because $\rho(\bar{X}/\hat{X}) = 1$). Since V is either $\mathbb{P}^1$, or a smooth del Pezzo surface, $S_2|_V = 0$ and $a_i \leq 3$. So, $r = 7$. By the above claim and computations in the table we have $a_2 = 3$, $m_1 = 1$, and $m_2 = 0$. Hence, $a_1 = 2$. But then

$$-K_V \sim 2\bar{E}|_V \sim 2\bar{S}_3|_V + 3\bar{E}|_V,$$

a contradiction.

Thus g is birational. Below we will use notation of 4.12. Since $\bar{S}_3$ is moveable, $s_3 \geq 1$. Put

$$u := s_2 + em_2, \qquad v := s_3 + em_3.$$

5.8. Case: $r = 11$. Since $\mathrm{Cl}(X)/\!\sim_{\mathbb{Q}} \simeq \mathbb{Z}\cdot\Theta$, pushing down (5.2) to $\hat{X}$ we obtain the following relations

$$\begin{aligned} \hat{q} &= 5s_2 + (4 + 5m_2)e &&= 5u + 4e, \\ \hat{q} &= 2s_2 + 2s_3 + (3 + 2m_2 + 2m_3)e &&= 2u + 2v + 3e. \end{aligned} \tag{5.9}$$

Assume that $u = 0$. Then $\hat{q} = 4e$. The only solution of (5.9) with $\hat{q}$ allowed by Proposition 3.6 is the following: $\hat{q} = 8$, $v = 1$, $e = 2$. Hence, $s_2 = 0$ and $s_3 = 1$. In particular, $\dim|\Theta| \geq \dim|S_3| = 1$. On the other hand, by Lemma 4.13 the group $\mathrm{Cl}(\hat{X})$ is torsion free and by Lemma 3.9 the divisor Θ is not moveable, a contradiction.

Therefore, $u \geq 1$. By the first relation in (5.9) $\hat{q} \geq 9$. Hence the group $\mathrm{Cl}(\hat{X})$ is torsion free (Proposition 3.6). Then by Lemma 4.13 we have $F \sim eA$. Since $|A| = \varnothing$, $e \geq 2$. Again by (5.9) $\hat{q} \geq 13$ and e is odd. Thus, $e = 3$, $u = 1$, and $\hat{q} = 17$. Further, $s_3 + em_3 = v = 3$ and $s_3 = 3$ (because $\bar{S}_3$ is moveable). By Proposition 3.6 we have $1 = \dim|S_3| \leq \dim|3\Theta| = 0$, a contradiction.

5.10. Case: $r = 7$. Recall that $m_3 \geq 1$ by Claim 5.7. As in 5.8 write

$$\begin{array}{rcccl} \hat{q} & = & 5s_2 + (2 + 5m_2)e & = & 5u + 2e, \\ \hat{q} & = & 2s_2 + 2s_3 + (1 + 2m_2 + 2m_3)e & = & 2u + 2v + e. \end{array} \tag{5.11}$$

Hence, $v = s_3 + em_3 \geq 1 + e$.

If $u = 0$, then $\hat{q} = 2e = 2v + e$, $e = 2v$, and $\hat{q} = 4v \geq 4(1 + e) = 4(1 + 2v)$, a contradiction. If $u = 2$, then $\hat{q}$ is even ≥ 12. Again we have a contradiction.

Assume that $u \geq 3$. Using the first relation in (5.11) and Proposition 3.6 we get successively

$$u = 3, \quad \hat{q} \geq 17, \quad |\Theta| = \varnothing, \quad e \geq 2, \quad \hat{q} \geq 19, \quad |2\Theta| = \varnothing, \quad e \geq 3,$$

and so $\hat{q} \geq 21$, a contradiction.

Therefore, $u = 1$. Then $\hat{q} = 5 + 2e = 2 + 2v + e$ and $2v = 3 + e = 2v \geq 2 + 2e$. So, $e = 1$, $v = 2$, $\hat{q} = 7$. Since $m_3 \geq 1$, $s_3 = v - em_3 = 1$. Hence, $\hat{S}_3 \sim_{\mathbb{Q}} \Theta$. Since $\dim|\hat{S}_3| \geq 1$, by (vi) of Theorem 1.4 we have $\hat{X} \simeq \mathbb{P}(1^2, 2, 3)$. In particular, the group $\mathrm{Cl}(\hat{X})$ is torsion free. By Lemma 4.13 the divisor F generates the group $\mathrm{Cl}(X)$. This contradicts $|A| = \varnothing$.

The last contradiction finishes the proof of (v) of Theorem 1.4.

6. Case $\mathrm{q}\mathbb{Q}(X) = 11$ and $\dim|-K_X| \geq 11$

In this section we consider the case $\mathrm{q}\mathbb{Q}(X) = 11$ and $\dim|-K_X| \geq 11$. By Proposition 3.6 the group $\mathrm{Cl}(X)$ is torsion free and $\mathbf{B} = (2, 3, 5)$. Recall that

$$\dim|A| = 0, \quad \dim|2A| = 1, \quad \text{and} \quad \dim|3A| = 2.$$

It is easy to see that, for $m = 1$, 2, and 3, general members $S_m \in |-mK_X|$ are irreducible. For $r = 2$, 3, 5, let P_r be a (unique) point of index r. In notation of §4, take $\mathscr{M} := |2A|$. By the above, $\mathscr{M}$ is a pencil without fixed components. Apply Construction (4.5). Near P_5 we have $A \sim -K_X$ and $\mathscr{M} \sim -2K_X$. By Lemma 4.2 we get $c \leq 1/2$. In particular, the pair $(X, \mathscr{M})$ is not canonical.

Proposition 6.1. *In the above notation, f is the Kawamata blowup of P_5 and $\hat{X}$ is a del Pezzo surface with Du Val singularities with $K_{\hat{X}}^2 = 5$ or 6. Moreover, for $k = 1$, 2 and 3, the image $C_k := g(\bar{S}_k)$ is a curve on $\hat{X}$ with $-K_{\hat{X}} \cdot C_k = k$.*

Proof. Similar to (5.2)-(5.3) we have for some $a_1, a_2, a_3 \in \mathbb{Z}$:

$$\begin{array}{lcl} K_{\bar{X}} + 11\bar{S}_1 + a_1\bar{E} & \sim & 0, \\ K_{\bar{X}} + \bar{S}_1 + 5\bar{S}_2 + a_2\bar{E} & \sim & 0, \\ K_{\bar{X}} + 2\bar{S}_1 + 3\bar{S}_3 + a_3\bar{E} & \sim & 0, \end{array} \tag{6.2}$$

$$\begin{array}{lrcl} & 11\beta_1 & = & a_1+\alpha, \\ (6.3) & \beta_1+5\beta_2 & = & a_2+\alpha, \\ & 2\beta_1+3\beta_3 & = & a_3+\alpha. \end{array}$$

Since $S_2 \in \mathscr{M}$ is a general member, by (4.9) we have $c = \alpha/\beta_2 \le 1/2$, so $2\alpha \le \beta_2$ and $a_2 \ge 9\alpha + \beta_1$. Since $2S_1 \sim S_2$, we have $2\beta_1 \ge \beta_2$. Thus $\beta_1 \ge \alpha$ and $a_1,\, a_2 \ge 10\alpha$.

First we consider the case where $f(E)$ is either a curve or a Gorenstein point on X. Then α and β_k are integers, so $a_1,\, a_2 \ge 10$. Restricting (6.2) to a general fiber of g we obtain that g is birational. Moreover, in notation of 4.12 we have $\hat{q} \ge 15$, the group $\mathrm{Cl}(\hat{X})$ is torsion free, and $\hat{E} \sim \Theta$. In particular, $|\Theta| \ne \varnothing$. This contradicts Proposition 3.6.

6.4. Therefore $P := f(E)$ is a non-Gorenstein point of index $r = 2, 3$ or 5. As in 5.6 we have the following values of β_k and a_k:

r	β_1	β_2	β_3	a_1	a_2	a_3
2	$\frac{1}{2}+m_1$	m_2	$\frac{1}{2}+m_3$	$5+11m_1$	m_1+5m_2	$2+2m_1+3m_3$
3	$\frac{2}{3}+m_1$	$\frac{1}{3}+m_2$	m_3	$7+11m_1$	$1+m_1+5m_2$	$1+2m_1+3m_3$
5	$\frac{1}{5}+m_1$	$\frac{2}{5}+m_2$	$\frac{3}{5}+m_3$	$2+11m_1$	$2+m_1+5m_2$	$2+2m_1+3m_3$

Claim 6.5. *If $r = 2$ or 3, then $m_2 \ge 1$.*

Proof. Follows from $1/2 \ge c = \alpha/\beta_2 = 1/r\beta_2$. □

Assume that g is birational. By Proposition 3.6 and Remark 4.10 we have $\dim|-K_{\hat{X}}| \ge |-K_X| = 23$. So, in notation of 4.12, $\hat{q} \le 11$. If $\bar{S}_1$ is not contracted, then by the first relation in (6.2) we have $\hat{q} \ge 11 + a_1 \ge 13$, a contradiction. Therefore the divisor $\bar{S}_1$ is contracted. By Lemma 4.13 the group $\mathrm{Cl}(\hat{X})$ is torsion free and $\hat{E} \sim \Theta$. Hence, $\hat{q} = a_1 \le 7$, $m_1 = 0$, and $r \ne 5$. But then $m_2 \ge 1$ (see Claim 6.5) and $a_2 \ge 5$. This contradicts the second relation in (6.2).

Therefore g is of fiber type. Restricting (6.2) to a general fiber we get $a_i \le 3$. Thus, $r = 5$ and $a_1 = a_2 = a_3 = 2$. Moreover, divisors $\bar{S}_1$, $\bar{S}_2$, and $\bar{S}_3$ are g-vertical. Since $\bar{S}_3$ is irreducible and $\dim|\bar{S}_3| = 2$, the variety $\hat{X}$ cannot be a curve. Therefore $\hat{X}$ is a surface and the images $g(\bar{S}_1)$, $g(\bar{S}_2)$, and $g(\bar{S}_3)$ are curves. Since $\dim|\bar{S}_1| = 0$, we have $\dim|g(\bar{S}_1)| = 0$. Hence, $K_{\hat{X}}^2 \le 6$ and $g(\bar{S}_1)$ is a line on $\hat{X}$. By Lemma 4.14 there are only two possibilities: $\hat{X} \simeq \mathbb{P}(1,2,3)$ and $\hat{X}$ is an A_4-del Pezzo surface. □

6.6. Consider the case where $\hat{X}$ is an A_4-del Pezzo surface. Assume that $\bar{S}_6$ is g-vertical. By Riemann-Roch for Weil divisors on surfaces with Du Val singularities [Rei87] we have $\dim|\bar{S}_6| = \dim|g(\bar{S}_6)| = 6$. On the other hand, $\dim|\bar{S}_6| = \dim|S_6| = 7$, a contradiction. Thus $g(\bar{S}_5) = \hat{X}$. Since $K_X + S_5 + S_6 \sim 0$,

$$K_{\bar{X}} + \bar{S}_5 + \bar{S}_6 + \bar{E} \sim 0.$$

Therefore $\bar{S}_6$ and $\bar{E}$ are sections of g. By Proposition 4.18 the pair $(\bar{X}, \bar{S}_6+\bar{E})$ is canonical. Now since $\bar{S}_5$ is nef, the map $\bar{X} \dashrightarrow \tilde{X}$ is a composition of steps of the $K_{\bar{X}}+\bar{S}_6+\bar{E}$-MMP. Hence the pair $(\tilde{X}, \tilde{S}_6+E)$ is also canonical. In particular, $\tilde{S}_6 \cap E = \varnothing$ and so $P_5 = f(E) \notin S_6$, a contradiction.

6.7. Now consider the case $\hat{X} \simeq \mathbb{P}(1,2,3)$. As above, if $g(\bar{S}_5)$ is a curve, then $\dim |g(\bar{S}_5)| = 5$ and $g(\bar{S}_5) \sim 5g(\bar{S}_1)$. On the other hand, $g(\bar{S}_5) \sim -\frac{5}{6}K_{\hat{X}}$. But then $\dim |g(\bar{S}_5)| = 4$, a contradiction. Therefore, $g(\bar{S}_5) = \hat{X}$. Similar to (6.2) we have $K_{\bar{X}} + 2\bar{S}_5 + \bar{S}_1 + a_4\bar{E} \sim 0$. This shows that $a_4 = 0$ and $\bar{S}_5$ is a section of g. Thus we can write $K_{\bar{X}} + \bar{S}_5 + G + \bar{E} \sim 0$, where G is a g-trivial Weil divisor, i.e., $G = g^*\Gamma$ for some Weil divisor Γ. Pushing down this equality to X we get $G \sim 6\bar{S}_1$, i.e., $\Gamma \in |-K_{\hat{X}}|$. By Proposition 4.18 varieties $\bar{X}$ and X are toric. This proves (iv) of Theorem 1.4.

7. Case $\mathrm{q}\mathbb{Q}(X) = 13$ and $\dim |-K_X| \geq 6$

In this section we consider the case $\mathrm{q}\mathbb{Q}(X) = 13$ and $\dim |-K_X| \geq 6$. By Proposition 3.6 $\mathbf{B} = (3,4,5)$. Recall that

$$\dim |A| = \dim |2A| = 0,\ \dim |3A| = 1,\ \dim |4A| = 2,\ \text{and}\ \dim |5A| = 3.$$

Therefore, for $m = 1$, 3, 4, and 5, general members $S_m \in |-mK_X|$ are irreducible. For $r = 3$, 4, 5, let P_r be a (unique) point of index r. In notation of §4, take $\mathscr{M} := |4A|$. Since $1 = \dim |3A| > \dim \mathscr{M} = 2$, the linear system $\mathscr{M}$ has no fixed components. Apply Construction (4.5). Near P_5 we have $A \sim -2K_X$ and $\mathscr{M} \sim -3K_X$. By Lemma 4.2 we get $c \leq 1/3$. In particular, the pair $(X, \mathscr{M})$ is not canonical.

Proposition 7.1. *In the above notation, f is the Kawamata blowup of P_5, g is birational, it contracts $\bar{S}_1$, and $\hat{X} \simeq \mathbb{P}(1^3, 2)$. Moreover, in notation of* 4.12 *we have $\hat{S}_3 \sim \hat{S}_4 \sim \hat{E} \sim \Theta$ and $\hat{S}_5 \sim 2\Theta$.*

Proof. Similar to (5.2)-(5.3) we have for some $a_1, a_2, a_3 \in \mathbb{Z}$:

$$\begin{array}{lll} K_{\bar{X}} + 13\bar{S}_1 + a_1\bar{E} & \sim & 0, \\ K_{\bar{X}} + \bar{S}_1 + 4\bar{S}_3 + a_2\bar{E} & \sim & 0, \\ K_{\bar{X}} + \bar{S}_1 + 3\bar{S}_4 + a_3\bar{E} & \sim & 0, \end{array} \tag{7.2}$$

$$\begin{array}{lll} 13\beta_1 & = & a_1 + \alpha, \\ \beta_1 + 4\beta_3 & = & a_2 + \alpha, \\ \beta_1 + 3\beta_4 & = & a_3 + \alpha. \end{array} \tag{7.3}$$

Since $S_4 \in \mathscr{M}$ is a general member, by (4.9) we have $c = \alpha/\beta_4 \leq 1/3$, $3\alpha \leq \beta_4$ and $a_3 \geq 8\alpha + \beta_1$. Since $4S_1 \sim S_4$, we have $4\beta_1 \geq \beta_4$. Thus $\beta_1 \geq \alpha$ and $a_1 \geq 12\alpha$.

First we consider the case where $f(E)$ is either a curve or a Gorenstein point on X. Then α and β_k are integers. In particular, $a_1 \geq 12$. From the first relation in (7.2) we obtain that g is birational. Moreover, in notation of 4.12

we have $\hat{q} \geq 13$ and $\hat{E} \sim \Theta$. In particular, $|\Theta| \neq \varnothing$. By Proposition 3.6 we have $\hat{q} = 13$, $a_1 = 13$, $\bar{S}_1$ is contracted, and $\alpha = 1$. This contradicts (7.3). Therefore $P := f(E)$ is a non-Gorenstein point of index $r = 3, 4$ or 5. By Theorem 4.11 $\alpha = 1/r$. Similar to 5.6 we have (here $m_k \in \mathbb{Z}_{\geq 0}$)

r	β_1	β_3	β_4	β_5	a_1	a_2	a_3
3	$\frac{1}{3}+m_1$	m_3	$\frac{1}{3}+m_4$	$\frac{2}{3}+m_5$	$4+13m_1$	m_1+4m_3	$1+m_1+3m_4$
4	$\frac{1}{4}+m_1$	$\frac{3}{4}+m_3$	m_4	$\frac{1}{4}+m_5$	$3+13m_1$	$3+m_1+4m_3$	m_1+3m_4
5	$\frac{2}{5}+m_1$	$\frac{1}{5}+m_3$	$\frac{3}{5}+m_4$	m_5	$5+13m_1$	$1+m_1+4m_3$	$2+m_1+3m_4$

Claim 7.4. *If $r = 3$ or 4, then $m_4 \geq 1$.*

Proof. Follows from $1/3 \geq c = \alpha/\beta_4 = 1/r\beta_4$. □

If g is not birational, then $a_1 = 3$, $r = 4$, $m_4 \geq 1$, and $a_3 \geq 3$. In this case, $a_2 = a_3 = 3$, g is a generically $\mathbb{P}^2$-bundle, and divisors $\bar{S}_1$, $\bar{S}_3$, $\bar{S}_4$ are g-vertical. Since $\dim|\bar{S}_4| > 1$ and the divisor $\bar{S}_4$ is irreducible, we have a contradiction. Therefore g is birational. Below we will use notation of 4.12.
By Proposition 3.6 we have $\dim|-K_{\hat{X}}| \geq |-K_X| = 19$ and $\hat{q} \leq 13$. From the first relation in (7.2) we see that $\bar{S}_1$ is contracted. By Lemma 4.13 the group $\mathrm{Cl}(\hat{X})$ is torsion free and $\hat{E} \sim \Theta$. Moreover, $m_1 = 0$ (because $13m_1 < a_1 e = \hat{q} \leq 13$). Thus $\hat{q} = a_1 = 4$, 3, and 5 in cases $r = 3$, 4, and 5, respectively.
In cases $r = 3$ and 4 we have $\hat{q} \geq 3 + a_3 \geq 6$, a contradiction. Therefore, $r = 5$, $\hat{q} = 5$, and $s_3 = s_4 = 1$. Since $\dim|\Theta| \geq 1$, by (vi) of Theorem 1.4 we have $\hat{X} \simeq \mathbb{P}(1^3, 2)$. Since $\dim|S_5| = 3$ and $\dim|\Theta| = 2$, $s_5 \geq 2$. Similar to (7.2)-(7.3) we have $K_{\bar{X}} + \bar{S}_3 + 2\bar{S}_5 + a_4\bar{E} \sim 0$, $2s_5 + a_4 = 4$, and $a_4 = \beta_3 + 2\beta_5 - \alpha = m_3 + 2m_5$. Thus, $s_5 = 2$ and $a_4 = \beta_5 = 0$, i.e., $P_5 \notin S_5$. □

Lemma 7.5. (i) *$S_1 \cap S_3$ is a reduced irreducible curve.*
(ii) *$S_1 \cap S_3 \cap S_4 = \{P_5\}$.*

Proof. (i) Recall that $A^3 = 1/60$ by Proposition 3.6. Write $S_1 \cap S_3 = C + \Gamma$, where C is a reduced irreducible curve passing through P_5 and Γ is an effective 1-cycle. Suppose, $\Gamma \neq 0$. Then $1/4 = S_1 \cdot S_3 \cdot S_5 > S_5 \cdot C$. Since $P_5 \notin S_5$, $C \not\subset S_5$ and $S_5 \cdot C \geq 1/4$, a contradiction. Hence, $S_1 \cap S_3 = C$.
(ii) Assume that $S_1 \cap S_3 \cap S_4 \ni P \neq P_5$. Since $1/5 = S_1 \cdot S_3 \cdot S_4 = S_4 \cdot C$ and P, $P_5 \in S_4 \cap C$, we have $C \subset S_4$. If there is a component $C' \neq C$ of $S_1 \cap S_4$ not contained in S_5, then, as above, $1/3 = S_1 \cdot S_4 \cdot S_5 \geq S_5 \cdot C + S_5 \cdot C' \geq 1/2$, a contradiction. Thus we can write $S_1 \cap S_4 = C + \Gamma$, where Γ is an effective 1-cycle with $\operatorname{Supp}\Gamma \subset S_5$. In particular, $P_5 \notin \Gamma$. The divisor $12A$ is Cartier at P_3 and P_4. We get

$$\frac{1}{5} = 12A^3 = 12A \cdot S_1 \cdot (S_4 - S_3) = 12A \cdot \Gamma \in \mathbb{Z},$$

a contradiction. □

Lemma 7.6. *Let X be a $\mathbb{Q}$-Fano threefold and $D = D_1 + \cdots + D_4$ be a divisor on X, where D_i are irreducible components. Let $P \in X$ be a cyclic quotient singularity of index r. Assume that $K_X + D \sim_{\mathbb{Q}} 0$, $P \notin D_4$, $D_1 \cap D_2 \cap D_3 = \{P\}$, and $D_1 \cdot D_2 \cdot D_3 = 1/r$. Then the pair (X, D) is LC.*

Proof. Let $\pi\colon (X^\sharp, P^\sharp) \to (X, P)$ be the index-one cover. For $k = 1, 2, 3$, let $D_k^\sharp$ be the preimage of D_k and let $D^\sharp := D_1^\sharp + D_2^\sharp + D_3^\sharp$. By our assumptions $D_1^\sharp \cap D_2^\sharp \cap D_3^\sharp = \{P^\sharp\}$. Since $D_1 \cdot D_2 \cdot D_3 = 1/r$, locally near $P^\sharp$ we have $D_1^\sharp \cdot D_2^\sharp \cdot D_3^\sharp = 1$. Hence $D^\sharp$ is a simple normal crossing divisor (near $P^\sharp$). In particular, $(X^\sharp, D^\sharp)$ is LC near $P^\sharp$ and so is (X, D) near P.
Thus the pair (X, D) is LC in some neighborhood $U \ni P$. Since $D_1 \cap D_2 \cap D_3 = \{P\}$, P is a center of LC singularities for (X, D). Let H be a general hyperplane section through P. Write $\lambda D_4 \sim_{\mathbb{Q}} H$, where $\lambda > 0$. If (X, D) is not LC in $X \setminus U$, then the locus of log canonical singularities of the pair $(X, D + \epsilon H - (\lambda\epsilon + \delta) D_4)$ is not connected for $0 < \delta \ll \epsilon \ll 1$. This contradicts Connectedness Lemma [Sho92], [Kol92]. Therefore the pair (X, D) is LC. □

7.7. Proof of (iii) of Theorem 1.4. By Lemma 7.6 the pair $(X, S_1 + S_3 + S_4 + S_5)$ is LC. Since $K_X + S_1 + S_3 + S_4 + S_5 \sim 0$, it is easy to see that $a(E, S_1 + S_3 + S_4 + S_5) = -1$. Thus $K_{\tilde{X}} + \tilde{S}_1 + \tilde{S}_3 + \tilde{S}_4 + \tilde{S}_5 = f^*(K_X + S_1 + S_3 + S_4 + S_5) \sim 0$. Therefore the pairs $(\bar{X}, \bar{S}_1 + \bar{S}_3 + \bar{S}_4 + \bar{S}_5 + \bar{E})$ and $(\hat{X}, \hat{S}_3 + \hat{S}_4 + \hat{S}_5 + \hat{E})$ are also LC. It follows from Proposition 7.1 and its proof that $\hat{X} \simeq \mathbb{P}(1^3, 2)$, $\hat{E} \sim \hat{S}_3 \sim \hat{S}_4 \sim \Theta$, and $\hat{S}_5 \sim 2\Theta$. We claim that $\hat{S}_3 + \hat{S}_4 + \hat{S}_5 + \hat{E}$ is a toric boundary (for a suitable choice of coordinates in $\mathbb{P}(1^3, 2)$). Let $(x_1 : x_1' : x_1'' : x_2)$ be homogeneous coordinates in $\mathbb{P}(1^3, 2)$. Clearly, we may assume that $\hat{E} = \{x_1 = 0\}$, $\hat{S}_3 = \{x_1' = 0\}$, and $\hat{S}_4 = \{\alpha x_1 + \alpha' x_1' + \alpha'' x_1'' = 0\}$ for some constants α, α', α''. Since $(\hat{X}, \hat{S}_3 + \hat{S}_4 + \hat{E})$ is LC, $\alpha'' \neq 0$ and after a coordinate change we may assume that $\hat{S}_4 = \{x_1'' = 0\}$. Further, the surface $\hat{S}_5$ is given by the equation $\beta x_2 + \psi(x_1, x_1', x_1'') = 0$, where β is a constant and ψ is a quadratic form. If $\beta = 0$, then $\hat{S}_3 \cap \hat{S}_4 \cap \hat{E} \cap \hat{S}_5 \neq \varnothing$ and the pair $(\hat{X}, \hat{S}_3 + \hat{S}_4 + \hat{S}_5 + \hat{E})$ cannot be LC. Thus $\beta \neq 0$ and after a coordinate change we may assume that $\hat{S}_5 = \{x_2 = 0\}$. Therefore $\hat{S}_3 + \hat{S}_4 + \hat{S}_5 + \hat{E}$ is a toric boundary. Then by Lemma 7.8 below the varieties $\bar{X}$, $\tilde{X}$, and X are toric. This proves (iii) of Theorem 1.4.

Lemma 7.8 (see, e.g., [McK01, 3.4]). *Let V be a toric variety and let Δ be the toric (reduced) boundary. Then every valuation ν with discrepancy -1 with respect to $K_V + \Delta$ is toric, that is, there is a birational toric morphism $\tilde{V} \to V$ such that ν corresponds to an exceptional divisor.*

8. Case $\mathrm{q}\mathbb{Q}(X) = 17$

Consider the case $\mathrm{q}\mathbb{Q}(X) = 17$. By Proposition 3.6 $\mathbf{B} = (2, 3, 5, 7)$ and $|A| = \varnothing$, $\dim|2A| = \dim|3A| = \dim|4A| = 0$, $\dim|5A| = \dim|6A| = 1$, $\dim|7A| = 2$. Therefore, for $m = 2$, 3, 5, and 7 general members $S_m \in |-mK_X|$ are irreducible. For $r = 2$, 3, 5, 7, let P_r be a (unique) point of index r. In notation of §4, take $\mathscr{M} := |5A|$ and apply Construction (4.5). Near P_7 we have $A \sim -5K_X$ and $\mathscr{M} \sim -4K_X$. By Lemma 4.2 we get $c \le 1/4$. In particular, the pair $(X, \mathscr{M})$ is not canonical.

Proposition 8.1. *In the above notation, f is the Kawamata blowup of P_7, g is birational, it contracts $\bar{S}_2$, and $\hat{X} \simeq \mathbb{P}(1^2, 2, 3)$. Moreover, in notation of 4.12 we have $\hat{S}_3 \sim \hat{S}_5 \sim \Theta$, $\hat{E} \sim 2\Theta$, and $\hat{S}_7 \sim 3\Theta$.*

Proof. Similar to (5.2)-(5.3) we have for some $a_1, a_2, a_3 \in \mathbb{Z}$:

$$\begin{aligned} K_{\bar{X}} + 7\bar{S}_2 + \bar{S}_3 + a_1\bar{E} &\sim 0, \\ K_{\bar{X}} + \bar{S}_2 + 5\bar{S}_3 + a_2\bar{E} &\sim 0, \\ K_{\bar{X}} + \bar{S}_2 + 3\bar{S}_5 + a_3\bar{E} &\sim 0, \end{aligned} \tag{8.2}$$

$$\begin{aligned} 7\beta_2 + \beta_3 &= a_1 + \alpha, \\ \beta_2 + 5\beta_3 &= a_2 + \alpha, \\ \beta_2 + 3\beta_5 &= a_3 + \alpha. \end{aligned} \tag{8.3}$$

Since $S_5 \in \mathscr{M}$ is a general member, by (4.9) we have $c = \alpha/\beta_5 \le 1/4$, so $4\alpha \le \beta_5$ and $a_3 \ge 11\alpha + \beta_2$. Since $S_2 + S_3 \sim S_5$, we have $\beta_2 + \beta_3 \ge \beta_5 \ge 4\alpha$. Hence, $a_1 \ge 6\beta_2 + 3\alpha$ and $a_2 \ge 4\beta_3 + 3\alpha$.

First we consider the case where $f(E)$ is either a curve or a Gorenstein point on X. Then α and β_k are integers. In particular, $a_3 \ge 11$ and by the third relation in (8.2) we obtain that g is birational. Moreover, in notation of 4.12 we have $\hat{q} \ge 11$. In particular, the group $\mathrm{Cl}(\hat{X})$ is torsion free and so $\hat{E} \ge 2\Theta$. Hence, $\hat{q} \ge 2a_3 \ge 22$, a contradiction.

Therefore $P := f(E)$ is a non-Gorenstein point of index $r = 2, 3, 5$ or 7. Similar to 5.6 we have $\alpha = 1/r$ and

r	β_2	β_3	β_5	β_7	a_1	a_2	a_3
2	m_2	$\frac{1}{2} + m_3$	$\frac{1}{2} + m_5$	$\frac{1}{2} + m_7$	$7m_2 + m_3$	$2 + m_2 + 5m_3$	$1 + m_2 + 3m_5$
3	$\frac{1}{3} + m_2$	m_3	$\frac{1}{3} + m_5$	$\frac{2}{3} + m_7$	$2 + 7m_2 + m_3$	$m_2 + 5m_3$	$1 + m_2 + 3m_5$
5	$\frac{1}{5} + m_2$	$\frac{4}{5} + m_3$	m_5	$\frac{1}{5} + m_7$	$2 + 7m_2 + m_3$	$4 + m_2 + 5m_3$	$m_2 + 3m_5$
7	$\frac{3}{7} + m_2$	$\frac{1}{7} + m_3$	$\frac{4}{7} + m_5$	m_7	$3 + 7m_2 + m_3$	$1 + m_2 + 5m_3$	$2 + m_2 + 3m_5$

Claim 8.4. (i) *If $r = 2$, then $m_5 \ge 2$ and $m_2 + m_3 \ge 2$.*
(ii) *If $r = 3$, then $m_5 \ge 1$ and $m_2 + m_3 \ge 1$.*
(iii) *If $r = 5$, then $m_5 \ge 1$.*

Proof. Note that $1/4 \ge c = \alpha/\beta_5 = 1/r\beta_5$ and $r\beta_5 \ge 4$. This gives us inequalities for m_5. The inequalities for $m_2 + m_3$ follows from $\beta_2 + \beta_3 \ge \beta_5$. □

From this we have $\min(a_1, a_2, a_3) \ge 3$. Moreover, the equality $\min(a_1, a_2, a_3) = 3$ holds only if $r = 7$. Therefore the contraction g can be of fiber type only if $a_1 = 3$, $r = 7$, $m_2 = m_3 = 0$, $\min(a_1, a_2, a_3) = 3$, $r = 7$, $m_2 = m_3 = m_5 = 0$, $a_3 = 2$, and $a_2 = 1$. Then g is a del Pezzo fibration of degree 9 and by the first relation in (8.2) divisors $\hat{S}_2$ and $\hat{S}_3$ are g-vertical. But then $a_2 = 3$, a

contradiction. From now on we assume that g is birational. Thus we use notation of 4.12 as usual.
Since $\bar{S}_5$ is moveable, it is not contracted. Therefore, $s_5 \geq 1$. By (8.2) we have

$$\begin{aligned} \hat{q} &= 7s_2 + s_3 + a_1 e, \\ \hat{q} &= s_2 + 5s_3 + a_2 e, \\ \hat{q} &= s_2 + 3s_5 + a_3 e. \end{aligned}$$

Put

$$u := s_2 + em_2, \qquad v := s_3 + em_3, \qquad w := s_5 + em_5.$$

8.5. Case: $r = 2$. Then $a_3 \geq 7$ and $\hat{q} \geq 3s_5 + a_3 \geq 10$. Hence the group $\mathrm{Cl}(\hat{X})$ is torsion free. So, $e \geq 2$ and $\hat{q} \geq 3s_5 + 2a_3 \geq 17$. In this case, $|\Theta| = \varnothing$. Therefore, $s_5 \geq 2$ and $\hat{q} \geq 3s_5 + 2a_3 \geq 20$, a contradiction.

8.6. Case: $r = 3$. Then

$$\begin{aligned} \hat{q} &= 7s_2 + s_3 + (2 + 7m_2 + m_3)e &= 7u + v + 2e, \\ \hat{q} &= s_2 + 5s_3 + (m_2 + 5m_3)e &= u + 5v, \\ \hat{q} &= s_2 + 3s_5 + (1 + m_2 + 3m_5)e &= u + 3w + e. \end{aligned}$$

Assume that $u > 0$. Then $\hat{q} \geq 9$. Hence the group $\mathrm{Cl}(\hat{X})$ is torsion free and $e \geq 2$. Since $\dim |S_5| = 1$ and $\dim |\Theta| \leq 0$, we have $s_5 \geq 2$. Since $m_5 \geq 1$ (see Claim 8.4), we have $w \geq 4$ and $\hat{q} > 13$. In this case, $s_5 \geq 5$, a contradiction.
Therefore, $u = 0$, $m_2 = 0$, $s_3 \neq 0$, $m_3 \geq 1$, and $v \geq 2$. So, $\hat{q} = 5v \geq 10$. Then we get a contradiction by (v) of Theorem 1.4.

8.7. Case: $r = 5$. Then

$$\begin{aligned} \hat{q} &= 7s_2 + s_3 + (2 + 7m_2 + m_3)e &= 7u + v + 2e, \\ \hat{q} &= s_2 + 5s_3 + (4 + m_2 + 5m_3)e &= u + 5v + 4e, \\ \hat{q} &= s_2 + 3s_5 + (m_2 + 3m_5)e &= u + 3w. \end{aligned}$$

From the first two relations we have $3u = 2v + e$ and $1 \leq u \leq 2$. Further, $\hat{q} - 4u = 3(v + e)$, so $\hat{q} \equiv u \mod 3$.
If $u = 2$, then e is even and $\hat{q} = 14 + v + 2e \geq 18$. So, $\hat{q} = 19$, a contradiction. Thus $u = 1$, $3 = 2v + e$, and $\hat{q} = 7 + v + 2e \geq 9$. By (v) of Theorem 1.4 $\hat{q}$ is odd. Hence, v is even, $e = 3$, $v = 0$, $\hat{q} = 13$. In this case, $s_5 + 3m_5 = w = 4$. By Claim 8.4 $m_5 = s_5 = 1$. Note that the group $\mathrm{Cl}(\hat{X})$ is torsion free and $s_2 = 1$. Thus $\dim |\Theta| > 0$. This contradicts Proposition 3.6.

8.8. Case: $r = 7$. Then

$$\begin{aligned} \hat{q} &= 7s_2 + s_3 + (3 + 7m_2 + m_3)e &= 7u + v + 3e, \\ \hat{q} &= s_2 + 5s_3 + (1 + m_2 + 5m_3)e &= u + 5v + e, \\ \hat{q} &= s_2 + 3s_5 + (2 + m_2 + 3m_5)e &= u + 3w + 2e. \end{aligned}$$

Assume that $u > 0$. Then $\hat{q} \geq 10$, the group $\mathrm{Cl}(\hat{X})$ is torsion free and so $e \geq 2$, $\hat{q} \geq 13$, $u = 1$. From the first two relations we get $\hat{q} + 2 = 7v$. Hence, $v = 3$, $\hat{q} = 19$, $e = 3$, and $s_2 = 0$. This contradicts the equality $1 = u = s_2 + em_2$.

Therefore, $u = 0$ and $s_2 = m_2 = 0$. From the first two relations we get $\hat{q} = 7v$. Thus, $\hat{q} = 7$, $v = 1$, $e = 2$, $w = 1$, $m_3 = m_5 = 0$, and $s_3 = s_5 = 1$. By Lemma 4.13 the group $\mathrm{Cl}(\hat{X})$ is torsion free and so $\dim|\Theta| \geq \dim|\bar{S}_5| > 0$. From (vi) of Theorem 1.4 we have $\hat{X} \simeq \mathbb{P}(1^2, 2, 3)$. In particular, $\dim|\Theta| = 1$. Further, similar to (8.2) we have

$$K_{\bar{X}} + \bar{S}_3 + 2\bar{S}_7 + a_4\bar{E} \sim 0,$$
$$\beta_3 + 2\beta_7 = a_4 + \alpha.$$

This gives us $a_4 = 2\beta_7$ and $s_7 + a_4 = 3$. Since $\dim|S_7| = 2$, $s_7 > 1$, $s_7 = 3$, $\hat{S}_7 \sim 3\Theta$, $a_4 = 0$, and $\beta_7 = 0$, i.e., $P_7 \notin S_7$.

□

Lemma 8.9. (i) *$S_2 \cap S_3$ is a reduced irreducible curve.*
(ii) *$S_2 \cap S_3 \cap S_5 = \{P_7\}$.*

Proof. (i) Similar to the proof of (i) of Lemma 7.5.
(ii) Put $C := S_3 \cap S_4$. Assume that $S_2 \cap S_3 \cap S_5 \ni P \neq P_7$. Since $1/7 = S_2 \cdot S_3 \cdot S_5 = S_5 \cdot C$ and P, $P_7 \in S_5 \cap C$, we have $C \subset S_5$. If there is a component $C' \neq C$ of $S_2 \cap S_5$ not contained in S_7, then, as above, $7/15 = S_2 \cdot S_7 \cdot S_7 \geq S_7 \cdot C + S_7 \cdot C' \geq 2/5$, a contradiction. Thus we can write $S_2 \cap S_5 = C + \Gamma$, where Γ is an effective 1-cycle with $\mathrm{Supp}\,\Gamma \subset S_7$. In particular, $P_7 \notin \Gamma$. The divisor $30A$ is Cartier at P_2, P_3, and P_5. We get

$$\frac{120}{210} = 120A^3 = 30A \cdot S_2 \cdot (S_5 - S_3) = 30A \cdot \Gamma \in \mathbb{Z},$$

a contradiction. □

Now the proof of (ii) of Theorem 1.4 can be finished similar to 7.7: the pair $(\hat{X}, \hat{S}_3 + \hat{S}_5 + \hat{E} + \hat{S}_7)$ is LC and the corresponding discrepancy of $\bar{S}_2$ is equal to -1.

9. Case $\mathrm{q}\mathbb{Q}(X) = 19$

Consider the case $\mathrm{q}\mathbb{Q}(X) = 19$. By Proposition 3.6 $\mathbf{B} = (3, 4, 5, 7)$ and $|A| = \varnothing$, $|2A| = \varnothing$, $\dim|3A| = \dim|4A| = \dim|5A| = \dim|6A| = 0$, $\dim|7A| = 1$. Therefore, for $m = 3$, 4, 5, and 7 general members $S_m \in |-mK_X|$ are irreducible. For $r = 3$, 4, 5, 7, let P_r be a (unique) point of index r. In notation of §4, take $\mathscr{M} := |7A| = |S_7|$ and apply Construction (4.5). Near P_5 we have $A \sim -4K_X$ and $\mathscr{M} \sim -3K_X$. By Lemma 4.2 we get $c \leq 1/3$. In particular, the pair $(X, \mathscr{M})$ is not canonical.

Proposition 9.1. *In the above notation, f is the Kawamata blowup of P_5, g is birational, it contracts $\bar{S}_3$, and $\hat{X} \simeq \mathbb{P}(1^2, 2, 3)$. Moreover, in notation of 4.12 we have $\hat{S}_4 \sim \hat{S}_7 \sim \Theta$, $\hat{E} \sim 3\Theta$, and $\hat{S}_5 \sim 2\Theta$.*

Proof. Similar to (5.2)-(5.3) we have for some $a_1, a_2, a_3, a_4 \in \mathbb{Z}$:

$$
\begin{array}{rcl}
K_{\bar{X}} + 5\bar{S}_3 + \bar{S}_4 + a_1\bar{E} & \sim & 0,\\
K_{\bar{X}} + \bar{S}_3 + 4\bar{S}_4 + a_2\bar{E} & \sim & 0,\\
K_{\bar{X}} + \bar{S}_4 + 3\bar{S}_5 + a_3\bar{E} & \sim & 0,\\
K_{\bar{X}} + \bar{S}_5 + 2\bar{S}_7 + a_4\bar{E} & \sim & 0,
\end{array} \tag{9.2}
$$

$$
\begin{array}{rcl}
5\beta_3 + \beta_4 & = & a_1 + \alpha,\\
\beta_3 + 4\beta_4 & = & a_2 + \alpha,\\
\beta_4 + 3\beta_5 & = & a_3 + \alpha,\\
\beta_5 + 2\beta_7 & = & a_4 + \alpha.
\end{array} \tag{9.3}
$$

Remark 9.4. Since $S_7 \in \mathscr{M}$ is a general member, by (4.9) we have $c = \alpha/\beta_7 \le 1/3$, so $3\alpha \le \beta_7$ and $a_4 \ge 5\alpha + \beta_5$. Further, $S_3 + S_4 \sim S_7$. Thus, $\beta_3 + \beta_4 \ge \beta_7 \ge 3\alpha$, $a_1 \ge 4\beta_3 + 2\alpha$, and $a_2 \ge 3\beta_4 + 2\alpha$.

Assume that $\hat{X}$ is a surface. Then $\hat{X}$ is such as in Lemma 4.14. From the first and second relations in (9.2) we obtain that S_3 and S_4 are g-vertical. Since $\dim|\bar{S}_k| = 0$, $\dim|g(\bar{S}_k)| = 0$, $k = 3, 4$. Hence, $K_{\hat{X}}^2 \le 6$ and the curves $g(\bar{S}_k)$ are in fact lines on $\hat{X}$. In particular, $g(\bar{S}_3) \sim g(\bar{S}_4)$. This implies $\bar{S}_3 \sim \bar{S}_4$ and $S_3 \sim S_4$, a contradiction.
Now assume that $\hat{X}$ is a curve and let G be a general fiber of g. Clearly, divisors $\bar{S}_3$ and $\bar{S}_4$ are g-vertical. If the divisor $\bar{S}_5$ is also g-vertical, then $k_3\bar{S}_3 \sim k_4\bar{S}_4 \sim k_5\bar{S}_5 \sim G$, where the k_i are the multiplicities of corresponding fibers. Considering proper transforms on X we get $3k_3 = 4k_4 = 5k_5$ and so $k_3 = 20k$, $k_4 = 14k$, $k_5 = 12k$ for some $k \in \mathbb{Z}$. This contradicts the main result of [MP08a]. Therefore the divisor $\bar{S}_5$ is g-horizontal. In this case, the degree of the general fiber is 9. As above we have $k_3\bar{S}_3 \sim k_4\bar{S}_4 \sim G$, $3k_3 = 4k_4$. So, $k_3 = 4k$, $k_4 = 3k$, $k \in \mathbb{Z}$. Again by [MP08a] g has no fibers of multiplicity divisible by 4.
From now on we assume that g is birational. Then in notation of 4.12,

$$\hat{q} = 5s_3 + s_4 + a_1e = s_3 + 4s_4 + a_2e = s_4 + 3s_5 + a_3e. \tag{9.5}$$

Consider the case where $f(E)$ is either a curve or a Gorenstein point on X. Then α and β_k are integers. By Remark 9.4

$$a_1 + a_2 = 5(\beta_3 + \beta_4) + \beta_3 - 2\alpha \ge 13\alpha \ge 13.$$

On the other hand, from (9.5) we obtain $2\hat{q} \ge 6s_3 + 5s_4 + 13 \ge 18$. So, $\hat{q} \ge 9$ (both $\bar{S}_3$ and $\bar{S}_4$ cannot be contracted). In this case, the group $\mathrm{Cl}(\hat{X})$ is torsion free and by Lemma 4.13 we have $\hat{E} \ge 3\Theta$. Since $a_4 \ge 5$, we have $\hat{E} \sim 3\Theta$, $\hat{q} \ge 15$, and $\bar{S}_3$ is contracted. In this situation, $|\Theta| = \varnothing$, so s_5, $s_7 \ge 2$. This contradicts the fourth relation in (9.2).

Therefore $P := f(E)$ is a non-Gorenstein point of index $r = 3, 4, 5$ or 7. Similar to 5.6 we have $\alpha = 1/r$ and

r	β_3	β_4	β_5	β_7	a_1	a_2	a_3
3	m_3	$\frac{1}{3}+m_4$	$\frac{2}{3}+m_5$	$\frac{1}{3}+m_7$	$5m_3+m_4$	$1+m_3+4m_4$	$2+m_4+3m_5$
4	$\frac{1}{4}+m_3$	m_4	$\frac{3}{4}+m_5$	$\frac{1}{4}+m_7$	$1+5m_3+m_4$	m_3+4m_4	$2+m_4+3m_5$
5	$\frac{2}{5}+m_3$	$\frac{1}{5}+m_4$	m_5	$\frac{3}{5}+m_7$	$2+5m_3+m_4$	$1+m_3+4m_4$	m_4+3m_5
7	$\frac{2}{7}+m_3$	$\frac{5}{7}+m_4$	$\frac{1}{7}+m_5$	m_7	$2+5m_3+m_4$	$3+m_3+4m_4$	$1+m_4+3m_5$

Claim 9.6. (i) *If $r = 3$ or 4, then $m_7 \ge 1$ and $m_3 + m_4 \ge 1$.*
(ii) *If $r = 7$, then $m_7 \ge 1$.*

Proof. To get inequalities for m_7 we use $1/3 \ge c = \alpha/\beta_7 = 1/r\beta_7$, $r\beta_7 \ge 3$. The inequalities for $m_3 + m_4$ follows from $\beta_3 + \beta_4 \ge \beta_7$. □

Thus, in all cases $a_1, a_2 \ge 1$. Put

$$u := s_3 + em_3, \qquad v := s_4 + em_4, \qquad w := s_5 + em_5.$$

9.7. Case: $r = 3$. Then $u + v > e(m_3 + m_4) \ge e$ by Claim 9.6. Further,

$$\begin{aligned} \hat{q} &= 5s_3 + s_4 + (5m_3 + m_4)e &&= 5u + v, \\ \hat{q} &= s_3 + 4s_4 + (1 + m_3 + 4m_4)e &&= u + 4v + e, \\ \hat{q} &= s_4 + 3s_5 + (2 + m_4 + 3m_5)e &&= v + 3w + 2e. \end{aligned}$$

If $u = 0$, then $v = \hat{q} = e + 4v$, a contradiction.
Assume that $u \ge 2$. Then $\hat{q} \ge 10$, $u \le 3$, the group $\mathrm{Cl}(\hat{X})$ is torsion free and by Lemma 4.13 we have $e \ge 3$. If $u = 2$, then $v \ge 2$, $\hat{q} \ge 13$, $v = \hat{q} - 10$, and $e \le \hat{q} - 2 - 4v \le 2$, a contradiction. If $u = 3$, then $v = 2$, $e = 6$, $\hat{q} = 17$, and $m_3 = m_4 = 0$. This contradicts Claim 9.6.
Therefore, $u = 1$. Then $v = \hat{q} - 5$, $19 = e + 3\hat{q}$, and $\hat{q} \le 6$. We get only one solution: $\hat{q} = 6$, $u = v = w = e = 1$. Recall that $m_3 + m_4 \ge 1$ by Claim 9.6. Hence either $s_3 = 0$ and $\hat{S}_4 \sim_{\mathbb{Q}} \hat{S}_5 \sim_{\mathbb{Q}} \hat{E} \sim_{\mathbb{Q}} \Theta$ or $s_4 = 0$ and $\hat{S}_3 \sim_{\mathbb{Q}} \hat{S}_5 \sim_{\mathbb{Q}} \hat{E} \sim_{\mathbb{Q}} \Theta$. In both cases $\hat{S}_5 \not\sim \hat{E}$ (otherwise $\bar{S}_5 \sim \bar{E} + l\bar{F}$ for some $l \in \mathbb{Z}$ and so $S_5 \sim lF$, a contradiction). Then we get a contradiction by Lemma 3.11.

9.8. Case: $r = 4$. As in the previous case, $u + v > e$ and

$$\begin{aligned} \hat{q} &= 5s_3 + s_4 + (1 + 5m_3 + m_4)e &&= 5u + v + e, \\ \hat{q} &= s_3 + 4s_4 + (m_3 + 4m_4)e &&= u + 4v. \end{aligned}$$

If u is even, then so is $\hat{q}$. Hence, $\hat{q} \le 10$. From the first relation we have $u = 0$, $\hat{q} = 4v$, and $e = 3v$. This contradicts $u + v > e$. Therefore u is odd.
Assume that $u = 1$. Then $\hat{q} = 5 + v + e = 1 + 4v$ and $e = 3v - 4$. Since $u + v > e$, there is only one possibility: $v = e = 2$, $\hat{q} = 9$. Then the group $\mathrm{Cl}(\hat{X})$ is torsion free. By Lemma 4.13 we have $F \in |2A| \ne \varnothing$, a contradiction.
Finally, assume $u \ge 3$. Then $u = 3$ and $\hat{q} = 15 + v + e = 3 + 4v \ge 16$. Thus, $\hat{q} = 19$, $v = 4$, and $e = 0$, a contradiction.

9.9. Case: $r = 7$. Then

$$\begin{array}{lllll} \hat{q} &=& 5s_3 + s_4 + (2 + 5m_3 + m_4)e &=& 5u + v + 2e, \\ \hat{q} &=& s_3 + 4s_4 + (3 + m_3 + 4m_4)e &=& u + 4v + 3e, \\ \hat{q} &=& s_4 + 3s_5 + (1 + m_4 + 3m_5)e &=& v + 3w + e. \end{array}$$

In this case, $u = (3v + e)/4 > 0$. Assume that $u \geq 2$. Then $\hat{q} \geq 13$ and the group $\mathrm{Cl}(\hat{X})$ is torsion free. By Lemma 4.13 we have $e \geq 3$. Further, $u = 2$, and $\hat{q} \geq 17$. We get $m_3 = 0$, $s_3 = 2$, $e \geq 4$, $\hat{q} = 19$, $e = 4$, and $v = 1$. This contradicts the last relation.
Therefore, $u = 1$. Then $3v + e = 4$. Assume that $e = 4$. Then $v = 0$, $\hat{q} = 13$, $w = 3$, $s_4 = 0$, $s_3 = 1$, and $m_4 = m_3 = 0$. Since $\dim|\Theta| = \dim|2\Theta| = 0$, we have $s_5 \geq 3$. Recall that $m_7 \geq 1$ by Claim 9.6. Hence, $\beta_7 \geq 1$ and $a_4 = 2\beta_7 \geq 2$. This contradicts the fourth relation in (9.2).
Therefore, $e < 4$. In this case, $e = 1$, $v = 1$, and $\hat{q} = 8$. Then $\hat{E} \sim_{\mathbb{Q}} \Theta$ and either $\hat{S}_3 \sim_{\mathbb{Q}} \Theta$ or $\hat{S}_4 \sim_{\mathbb{Q}} \Theta$ (because $u = v = 1$). This contradicts (vi) of Theorem 1.4.

9.10. Case: $r = 5$. From (9.2) we obtain

$$\begin{array}{lllll} \hat{q} &=& 5s_3 + s_4 + (2 + 5m_3 + m_4)e &=& 5u + v + 2e, \\ \hat{q} &=& s_3 + 4s_4 + (1 + m_3 + 4m_4)e &=& u + 4v + e, \\ \hat{q} &=& s_4 + 3s_5 + (m_4 + 3m_5)e &=& v + 3w. \end{array} \tag{9.11}$$

Then $e = 3v - 4u$. If $u \geq 2$, then $e = 3v - 4u \leq 3v - 6$, and so $v \geq 3$. Hence, $\hat{q} \geq 15$ and the group $\mathrm{Cl}(\hat{X})$ is torsion free. By Lemma 4.13 we have $e \geq 3$. So $\hat{q} = 19$, $e = 3$, $s_3 = 0$, and $2 = u = em_3 \geq 3$, a contradiction.
Assume that $u = 1$, then $e = 3v - 4$ and $v \geq 2$. Further, $\hat{q} = 7v - 3 = v + 3w \leq 19$. We get $\hat{q} = 11$ and $e = 2$. This contradicts Lemma 4.13.
Therefore, $u = 0$. Then $e = 3v$, $\hat{q} = 7v = 7$, $v = 1$, $e = 3$, and $w = 2$. By Lemma 4.13 the group $\mathrm{Cl}(\hat{X})$ is torsion free. Thus $s_3 = 0$, i.e., $\bar{S}_3$ is contracted, $s_4 = 1$, $s_5 = 2$, and $m_5 = \beta_5 = 0$. This means, in particular, that $P_5 \notin S_5$. From the fourth relation in (9.2) we get $a_4 = 1$ and $s_7 = 1$. In particular, $\dim|\Theta| > 0$ and $\hat{X} \simeq \mathbb{P}(1^2, 2, 3)$ by (vi) of Theorem 1.4.

□

Lemma 9.12. (i) *$S_3 \cap S_4$ is a reduced irreducible curve.*
(ii) *$S_3 \cap S_4 \cap S_7 = \{P_5\}$.*

Proof. (i) Similar to the proof of (i) of Lemma 7.5.
(ii) Put $C := S_3 \cap S_4$. Assume that $S_3 \cap S_4 \cap S_7 \ni P \neq P_5$. Since $1/5 = S_3 \cdot S_4 \cdot S_7 = S_7 \cdot C$ and P, $P_5 \in S_7 \cap C$, we have $C \subset S_7$. If there is a component $C' \neq C$ of $S_3 \cap S_7$ not contained in S_5, then, as above, $1/4 = S_3 \cdot S_7 \cdot S_5 \geq S_5 \cdot C + S_5 \cdot C' \geq 2/7$, a contradiction. Thus we can write $S_3 \cap S_7 = C + \Gamma$, where Γ is an effective 1-cycle with $\operatorname{Supp}\Gamma \subset S_5$. In particular, $P_5 \notin S_5$. The divisor $84A$ is Cartier at P_3, P_4, and P_7. We get

$$\frac{9}{5} = 84A \cdot S_3 \cdot (S_7 - S_4) = 84A \cdot \Gamma \in \mathbb{Z},$$

a contradiction. □

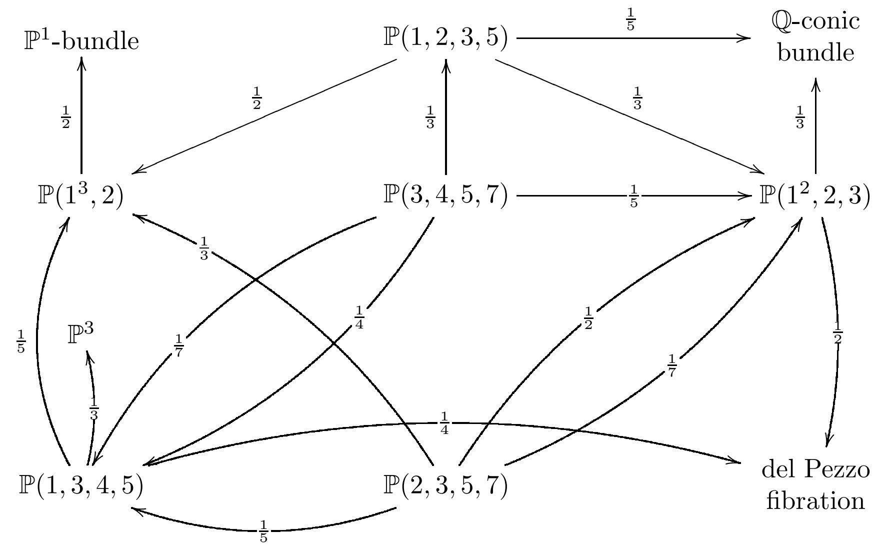
Now the proof of (i) of Theorem 1.4 can be finished similar to 7.7.

10. Toric Sarkisov links

Proposition 10.1. *Let X be a toric $\mathbb{Q}$-Fano threefold and let $P \in X$ be a cyclic quotient singularity of index r. Let $f\colon \tilde{X} \to X$ be the Kawamata blowup of $P \in X$. Then a general member of $|-K_X|$ is a normal surface having at worst Du Val singularities. The linear system $|-K_X|$ has only isolated base points. In particular, $-K_{\tilde{X}}$ is nef and big. The map $f\colon \tilde{X} \to X$ can be completed by a toric Sarkisov link* (*cf.* (4.5)).

Proof. This can be shown by explicit computations in all cases of Proposition 1.3. Consider, for example, the case $X = \mathbb{P}(3,4,5,7)$. Let x_3, x_4, x_5, x_7 be quasi-homogeneous coordinates in $\mathbb{P}(3,4,5,7)$. A section $S \in |-K_X|$ is given by a quasi-homogeneous polynomial of degree 19. By taking this polynomial as a general linear combination of $x_3^5x_4$, $x_3^3x_5^2$, $x_3^4x_7$, $x_4x_5^3$, $x_4^3x_7$, $x_5x_7^2$ we see that the base locus of $|-K_X|$ is the union of four coordinate points and the surface S has only quotient singularities. Since K_S is Cartier, the singularities of S are Du Val. Further, we can write $K_{\tilde{X}} + \tilde{S} = f^*(K_X + S) \sim 0$, where $\tilde{S}$ is the proper transform of S. Hence, $\tilde{S} \in |-K_{\tilde{S}}|$ and the linear system $|-K_{\tilde{X}}|$ has only isolated base points outside of $f^{-1}(P)$. In particular, $-K_{\tilde{X}}$ is nef. It is easy to check that $-K_{\tilde{X}}^3 > 0$, i.e., $-K_{\tilde{X}}$ is big. Recall that $\rho(\tilde{X}) = 2$. So, the Mori cone $\mathrm{NE}(\tilde{X})$ has exactly two extremal rays, say R_1 and R_2. Let R_1 is generated by f-exceptional curves. If $-K_{\tilde{X}}$ is ample, we run the MMP starting from R_2. Otherwise we make a flop in R_2 and run the MMP. Clearly, we obtain Sarkisov link (4.5). □

Explicitly, for weighted projective spaces from Proposition 1.3, we have the following diagram of Sarkisov links. Here an arrow $X_1 \xrightarrow{\frac{1}{r}} X_2$ indicates that there is a Sarkisov link described above that starts from the Kawamata blowup of a cyclic quotient singularity of index $r > 1$ on X_1 and the target variety is X_2.



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On Reductions of Families of Crystalline Galois Representations

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Abstract. Let K_f be the finite unramified extension of $\mathbb{Q}_p$ of degree f and E any finite large enough coefficient field containing K_f. We construct analytic families of étale (φ, Γ)-modules which give rise to families of crystalline E-representations of the absolute Galois group G_{K_f} of K_f. For any irreducible effective two-dimensional crystalline E-representation of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$ induced from a crystalline character of $G_{K_{2f}}$, we construct an infinite family of crystalline E-representations of G_{K_f} of the same Hodge-Tate type which contains it. As an application, we compute the semisimplified mod p reductions of the members of each such family.

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Contents

1 Introduction

Let p be a prime number and $\bar{\mathbb{Q}}_p$ a fixed algebraic closure of $\mathbb{Q}_p$. Let N be a positive integer and $g = \sum\limits_{n\geq 1} a_n q^n$ a newform of weight $k \geq 2$ over $\Gamma_1(N)$ with character ψ. The complex coefficients a_n are algebraic over $\mathbb{Q}$ and may be viewed as elements of $\bar{\mathbb{Q}}_p$ after fixing embeddings $\bar{\mathbb{Q}} \to \mathbb{C}$ and $\bar{\mathbb{Q}} \to \bar{\mathbb{Q}}_p$. By work of Eichler-Shimura when $k = 2$ and Deligne when $k > 2$, there exists a continuous irreducible two-dimensional p-adic representation $\rho_g : G_{\mathbb{Q}} \longrightarrow \mathrm{GL}_2(\bar{\mathbb{Q}}_p)$ attached to g. If $l \nmid pN$, then ρ_g is unramified at l and $\det(X - \rho_g(\mathrm{Frob}_l)) = X^2 - a_l X + \psi(l)\, l^{k-1}$, where Frob_l is any choice of an arithmetic Frobenius at l. The contraction of the maximal ideal of the ring of integers of $\bar{\mathbb{Q}}_p$ via an embedding $\bar{\mathbb{Q}} \to \bar{\mathbb{Q}}_p$ gives rise to the choice of a place of $\bar{\mathbb{Q}}$ above p, and the decomposition group D_p at this place is isomorphic to the local Galois group $G_{\mathbb{Q}_p}$ via the same embedding. The local representation

$$\rho_{g,p} : G_{\mathbb{Q}_p} \longrightarrow \mathrm{GL}_2(\bar{\mathbb{Q}}_p),$$

obtained by restricting ρ_g to D_p, is de Rham with Hodge-Tate weights $\{0, k-1\}$ ([Tsu99]). If $p \nmid N$ the representation $\rho_{g,p}$ is crystalline and the characteristic polynomial of Frobenius of the weakly admissible filtered φ-module $\mathbb{D}_{k,a_p} := \mathbb{D}_{\mathrm{cris}}(\rho_{g,p})$ attached to $\rho_{g,p}$ by Fontaine is $X^2 - a_p X + \psi(p)\, p^{k-1}$ ([Fal89] and [Sc90]). The roots of Frobenius are distinct if $k = 2$ and conjecturally distinct if $k \geq 3$ (see [CE98]). In this case, weak admissibility imposes a unique up to isomorphism choice of the filtration of $\mathbb{D}_{k,a_p}$, and the isomorphism class of the crystalline representation $\rho_{g,p}$ is completely determined by the characteristic polynomial of Frobenius of $\mathbb{D}_{k,a_p}$. The mod p reduction $\bar{\rho}_{g,p} : G_{\mathbb{Q}_p} \longrightarrow \mathrm{GL}_2(\bar{\mathbb{F}}_p)$ of the local representation $\rho_{g,p}$ is well defined up to semisimplification and plays a role in the proof of Serre's modularity conjecture, now a theorem of Khare and Wintenberger [KW09a], [KW09b], which states that any irreducible continuous odd Galois representation $\rho : G_{\mathbb{Q}} \longrightarrow \mathrm{GL}_2(\bar{\mathbb{F}}_p)$ is similar to a representation of the form $\bar{\rho}_g$ for a certain newform g which should occur in level $N(\rho)$, an integer prime-to-p, and weight $\kappa(\rho) \geq 2$, which Serre explicitly defined in [Ser87]. If $\rho_{g,p}$ is crystalline, the semisimplified mod p reduction $\bar{\rho}_{g,p}$ has been given concrete descriptions in certain cases by work of Berger-Li-Zhu [BLZ04] combined with work of Breuil [Bre03], which extended previous results of Deligne, Fontaine, Serre and Edixhoven, and more recently by Buzzard-Gee [BG09] using the p-adic Langlands correspondence for $\mathrm{GL}_2(\mathbb{Q}_p)$. For a more detailed account and the shape of these reductions see [Ber10, §5.2].

Recall that (up to unramified twist) all irreducible two-dimensional crystalline representations of $G_{\mathbb{Q}_p}$ with fixed Hodge-Tate weights in the range $[0;\ p]$ have the same irreducible mod p reduction. Reductions of crystalline representations of $G_{\mathbb{Q}_{p^f}} := \mathrm{Gal}(\bar{\mathbb{Q}}_p/\mathbb{Q}_{p^f})$ with $f \neq 1$, where $\mathbb{Q}_{p^f}$ is the unramified extension of $\mathbb{Q}_p$ of degree f, are more complicated. For example, in the simpler case where $f = 2$, there exist irreducible two-dimensional crystalline representation of $G_{\mathbb{Q}_{p^2}}$ with Hodge-Tate weights in the range $[0;\ p-1]$ sharing the same characteristic polynomial and filtration, with distinct irreducible or reducible reductions (cf. Proposition 6.22).

The purpose of this paper is to extend the constructions of [BLZ04] to two-dimensional crystalline representations of $G_{\mathbb{Q}_{p^f}}$, and to compute the semisimplified mod p reductions of the crystalline representations constructed. The strategy for computing reductions is to fit irreducible representations of G_{K_f} which are not induced from crystalline characters of $G_{K_{2f}}$ into families of representations of the same Hodge-Tate type and with the same mod p reduction, which contain some member which is either reducible or irreducible induced.

Serre's conjecture has been recently generalized by Buzzard, Diamond and Jarvis [BDJ] for irreducible totally odd two-dimensional $\bar{\mathbb{F}}_p$-representations of the absolute Galois group of any totally real field unramified at p, and has subsequently been extended by Schein [Sch08] to cases where p is odd and tamely ramified in F. Crystalline representations of the absolute Galois group of finite unramified extensions of $\mathbb{Q}_p$ arise naturally in this context of the conjecture of Buzzard, Diamond and Jarvis, and their modulo p reductions are crucial for the weight part of this conjecture (see [BDJ, §3]).

Let F be a totally real number field of degree $d > 1$, and let $I = \{\tau_1, ..., \tau_d\}$ be the set of real embeddings of F. Let $\mathbf{k} = (k_{\tau_1}, k_{\tau_2}, ..., k_{\tau_d}, w) \in \mathbb{N}_{\geq 1}^{d+1}$ with $k_{\tau_i} \equiv w \bmod 2$. We denote by $\mathcal{O}$ the ring of integers of F and we let $\mathfrak{n} \neq 0$ be an ideal of $\mathcal{O}$. The space $\mathrm{S}_{\mathbf{k}}(\mathrm{U}_1(\mathfrak{n}))$ of Hilbert modular cusp forms of level $\mathfrak{n}$ and weight $\mathbf{k}$ is a finite dimensional complex vector space endowed with actions of Hecke operators $\mathrm{T}_{\mathfrak{q}}$ indexed by the nonzero ideals $\mathfrak{q}$ of $\mathcal{O}$ (for the precise definitions see [Tay89]). Let $0 \neq g \in \mathrm{S}_{\mathbf{k}}(\mathrm{U}_1(\mathfrak{n}))$ be an eigenform for all the $\mathrm{T}_{\mathfrak{q}}$, and fix embeddings $\bar{\mathbb{Q}} \to \mathbb{C}$ and $\bar{\mathbb{Q}} \to \bar{\mathbb{Q}}_p$. By constructions of Rogawski-Tunnell [RT83], Ohta [Oht84], Carayol [Car86], Blasius-Rogawski [BR89], Taylor [Tay89], and Jarvis [Jar97], one can attach to g a continuous Galois representation $\rho_g : G_F \to \mathrm{GL}_2(\bar{\mathbb{Q}}_p)$, where G_F is the absolute Galois group of the totally real field F. Fixing an isomorphism between the residue field of $\bar{\mathbb{Q}}_p$ with $\bar{\mathbb{F}}_p$, the mod p reduction $\bar{\rho}_g : G_F \to \mathrm{GL}_2(\bar{\mathbb{F}}_p)$ is well defined up to semisimplification. A continuous representation $\rho : G_F \longrightarrow \mathrm{GL}_2(\bar{\mathbb{F}}_p)$ is called modular if $\rho \sim \bar{\rho}_g$ for some Hilbert modular eigenform g. Conjecturally, every irreducible totally odd continuous Galois representation $\rho : G_F \longrightarrow \mathrm{GL}_2(\bar{\mathbb{F}}_p)$ is modular ([BDJ]). We now assume that $k_{\tau_i} \geq 2$ for all i. We fix an isomorphism

$\bar{\mathbb{Q}}_p \overset{i}{\simeq} \mathbb{C}$ and an algebraic closure $\bar{F}$ of F. For each prime ideal $\mathfrak{p}$ of $\mathcal{O}$ lying above p we denote by $F_\mathfrak{p}$ the completion of F at $\mathfrak{p}$, and we fix an algebraic closure $\bar{F}_\mathfrak{p}$ of $F_\mathfrak{p}$ and an F-embedding $\bar{F} \hookrightarrow \bar{F}_\mathfrak{p}$. These determine a choice of a decomposition group $D_\mathfrak{p} \subset G_F$ an isomorphism $D_\mathfrak{p} \simeq G_{F_\mathfrak{p}}$. For each embedding $\tau : F_\mathfrak{p} \to \bar{\mathbb{Q}}_p$, let k_τ be the weight of g corresponding to the embedding $\tau_{|F} : F \to \bar{\mathbb{Q}}_p \overset{i}{\simeq} \mathbb{C}$. By works of Blasius-Rogawski [BR93], Saito [Sai09], Skinner [Ski09], and T. Liu [Liu09], the local representation $\rho_{g,F_\mathfrak{p}} : G_{F_\mathfrak{p}} \longrightarrow \mathrm{GL}_2(\bar{\mathbb{Q}}_p)$, obtained by restricting ρ_g to the decomposition subgroup $G_{F_\mathfrak{p}}$, is de Rham with labeled Hodge-Tate weights $\{\frac{k-k_\tau}{2}, \frac{k+k_\tau-2}{2}\}_{\tau:F_\mathfrak{p}\to\bar{\mathbb{Q}}_p}$, where $k = \max\{k_{\tau_i}\}$. This has also been proved by Kisin [Kis08, Theorem 4.3] under the assumption that $\rho_{g,F_\mathfrak{p}}$ is residually irreducible. If p is odd, unramified in F and prime to $\mathfrak{n}$, then $\rho_{g,F_\mathfrak{p}}$ is crystalline by works of Breuil [Bre99, Théorème 1(1)] and Berger [Ber04a, Théorème IV.2.1].

In the newform case, assuming that $\rho_{g,p}$ is crystalline, the weight of g and the eigenvalue of the Hecke operator T_p on g completely determine the structure of the filtered φ-module $\mathbb{D}_{\mathrm{cris}}(\rho_{g,p})$. In the Hilbert modular newform case, assuming that $\rho_{g,F_\mathfrak{p}}$ is crystalline, the structure of $\mathbb{D}_{\mathrm{cris}}(\rho_{g,F_\mathfrak{p}})$ is more complicated and the characteristic polynomial of Frobenius and the labeled Hodge-Tate weights do not suffice to completely determine its structure. The filtration of $\mathbb{D}_{\mathrm{cris}}(\rho_{g,F_\mathfrak{p}})$ is generally unknown, and, even worse, the characteristic polynomial of Frobenius and the filtration are not enough to determine the structure of the filtered φ-module $\mathbb{D}_{\mathrm{cris}}(\rho_{g,F_\mathfrak{p}})$. In this case, the isomorphism class is (roughly) determined by an extra parameter in $\left(\bar{\mathbb{Q}}_p^\times\right)^{f_\mathfrak{p}-1}$ (for a precise statement see [Dou10, §§6, 7]). As a consequence, if $f_\mathfrak{p} \geq 2$ there exist infinite families of non-isomorphic, irreducible two-dimensional crystalline representations of $G_{\mathbb{Q}_{p^{f_\mathfrak{p}}}}$ sharing the same characteristic polynomial and filtration.

For higher-dimensional crystalline E-representations of $G_{\mathbb{Q}_{p^f}}$, we mention that even in the simpler case of three-dimensional crystalline representations of $G_{\mathbb{Q}_p}$, there exist non-isomorphic Frobenius-semisimple crystalline representations sharing the same characteristic polynomial and filtration, with the same mod p reductions with respect to appropriately chosen Galois-stable $\mathcal{O}_E$-lattices. This follows by applying the constructions of §4 to the higher-dimensional case, and a proof is not included in this paper.

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1.1 PRELIMINARIES AND STATEMENT OF RESULTS

Throughout this paper p will be a fixed prime number, $K_f = \mathbb{Q}_{p^f}$ the finite unramified extension of $\mathbb{Q}_p$ of degree f, and E a finite large enough extension of

K_f with maximal ideal $\mathfrak{m}_E$ and residue field k_E. We simply write K whenever the degree over $\mathbb{Q}_p$ plays no role. We denote by σ_K the absolute Frobenius of K. We fix once and for all an embedding $K \overset{\tau_0}{\hookrightarrow} E$ and we let $\tau_j = \tau_0 \circ \sigma_K^j$ for all $j = 0, 1, ..., f-1$. We fix the f-tuple of embeddings $\mid \tau \mid := (\tau_0, \tau_1, ..., \tau_{f-1})$ and we denote $E^{|\tau|} := \prod_{\tau : K \hookrightarrow E} E$. The map $\xi : E \otimes K \to E^{|\tau|}$ with $\xi_K(x \otimes y) = (x\tau(y))_\tau$ and the embeddings ordered as above is a ring isomorphism. The ring automorphism $1_E \otimes \sigma_K : E \otimes K \to E \otimes K$ transforms via ξ to the automorphism $\varphi : E^{|\tau|} \to E^{|\tau|}$ with $\varphi(x_0, x_1, ..., x_{f-1}) = (x_1, ..., x_{f-1}, x_0)$. We denote by $e_j = (0, ..., 1, ..., 0)$ the idempotent of $E^{|\tau|}$ where the 1 occurs in the τ_j-th coordinate for each $j \in \{0, 1, ..., f-1\}$.

It is well-known (see for instance [BM02, Lemme 2.2.1.1]) that every continuous representation $\rho : G_K \to \mathrm{GL}_n(\bar{\mathbb{Q}}_p)$ is defined over some finite extension of $\mathbb{Q}_p$. Let $\rho : G_K \to \mathrm{GL}_E(V)$ be a continuous E-linear representation. Recall that $\mathbb{D}_{\mathrm{cris}}(V) = (\mathbb{B}_{\mathrm{cris}} \otimes_{\mathbb{Q}_p} V)^{G_K}$, where $\mathbb{B}_{\mathrm{cris}}$ is the ring constructed by Fontaine in [Fon88], is a filtered φ-module over K with E-coefficients, and V is crystalline if and only if $\mathbb{D}_{\mathrm{cris}}(V)$ is free over $E \otimes K$ of rank $\dim_E V$. One can easily prove that V is crystalline as an E-linear representation of G_K if and only if it is crystalline as a $\mathbb{Q}_p$-linear representation of G_K (cf. [CDT99] appendix B). We may therefore extend E whenever appropriate without affecting crystallinity. By a variant of the fundamental theorem of Colmez and Fontaine ([CF00], Théorème A) for nontrivial coefficients, the functor $V \mapsto \mathbb{D}_{\mathrm{cris}}(V)$ is an equivalence of categories from the category of crystalline E-linear representations of G_K to the category of weakly admissible filtered φ-modules $(\mathbb{D}, \varphi)$ over K with E-coefficients (see [BM02], §3). Such a filtered module $\mathbb{D}$ is a module over $E \otimes K$ and may be viewed as a module over $E^{|\tau|}$ via the ring isomorphism ξ defined above. Its Frobenius endomorphism is bijective and semilinear with respect to the automorphism φ of $E^{|\tau|}$. For each embedding τ_i of K into E we define $\mathbb{D}_i := e_i \mathbb{D}$. We have the decomposition $\mathbb{D} = \bigoplus_{i=0}^{f-1} \mathbb{D}_i$, and we filter each component $\mathbb{D}_i$ by setting $\mathrm{Fil^j}\mathbb{D}_i := e_i \mathrm{Fil^j}\mathbb{D}$. An integer j is called a labeled Hodge-Tate weight with respect to the embedding τ_i of K in E if and only if $e_i \mathrm{Fil^{-j}}\mathbb{D} \neq e_i \mathrm{Fil^{-j+1}}\mathbb{D}$ and is counted with multiplicity $\dim_E \left(e_i \mathrm{Fil^{-j}}\mathbb{D} / e_i \mathrm{Fil^{-j+1}}\mathbb{D} \right)$. Since the Frobenius endomorphism of $\mathbb{D}$ restricts to an E-linear isomorphism from $\mathbb{D}_i$ to $\mathbb{D}_{i-1}$ for all i, the components $\mathbb{D}_i$ are equidimensional over E. As a consequence, there are $n = \mathrm{rank}_{E \otimes K}(\mathbb{D})$ labeled Hodge-Tate weights for each embedding, counting multiplicities. The labeled Hodge-Tate weights of $\mathbb{D}$ are by definition the f-tuple of multisets $(W_i)_{\tau_i}$, where each such multiset W_i contains n integers, the opposites of the jumps of the filtration of $\mathbb{D}_i$. For crystalline characters we usually write $(-k_0, -k_1, ..., -k_{f-1})$ instead of $\{-k_i\}_{\tau_i}$. The characteristic polynomial of a crystalline E-linear representation of G_K is the characteristic polynomial of the $E^{|\tau|}$-linear map φ^f, where $(\mathbb{D}, \varphi)$ is the weakly admissible filtered φ-module corresponding to it by Fontaine's functor.

Definition 1.1. *A filtered φ-module $(\mathbb{D}, \varphi)$ is called F-semisimple, non-F-*

semisimple, or F-scalar if the $E^{|\tau|}$-linear map φ^f has the corresponding property.

We may twist $\mathbb{D}$ by some appropriate rank one weakly admissible filtered φ-module (see Proposition 3.5) and assume that $W_i = \{-w_{in-1} \leq ... \leq -w_{i2} \leq -w_{i1} \leq 0\}$ for all $i = 0, 1, ..., f-1$, for some non-negative integers w_{ij}. The Hodge-Tate weights of a crystalline representation V are the opposites of the jumps of the filtration of $\mathbb{D}_{\text{cris}}(V)$. If they are all non-positive, the crystalline representation is called effective or positive. To avoid trivialities, throughout the paper we assume that at least one labeled Hodge-Tate weight is strictly negative.

NOTATION 1.2. *Let k_i be nonnegative integers which we call weights. Assume that after ordering them and omitting possibly repeated weights we get $w_0 < w_1 < ... < w_{t-1}$, where w_0 is the smallest weight, w_1 the second smallest weight,..., and w_{t-1}, for some $1 \leq t \leq f$, is the largest weight. The largest weight w_{t-1} will be usually denoted by k. For convenience we define $w_{-1} = 0$. Let $I_0 = \{0, 1, ..., f-1\}$ and $I_0^+ = \{i \in I_0 : k_i > 0\}$. For $j = 1, 2, ..., t-1$ we let $I_j = \{i \in I_0 : k_i > w_{j-1}\}$ and for $j = t$ we define $I_t = \varnothing$. Let $f^+ = \left|I_0^+\right|$ be the number of strictly positive weights.*
For each subset $J \subset I_0$ we write $f_J = \sum\limits_{i \in J} e_i$ and $E^{|\tau_J|} = f_J \cdot E^{|\tau|}$. We may visualize the sets $E^{|\tau_{I_j}|}$ as follows: $E^{|\tau_{I_0}|}$ is the Cartesian product E^f. Starting with $E^{|\tau_{I_0}|}$, we obtain $E^{|\tau_{I_1}|}$ by killing the coordinates where the smallest weight occurs i.e. by killing the i-th coordinate for all i with $k_i = w_0$. We obtain $E^{|\tau_{I_2}|}$ by further killing the coordinates where the second smallest weight w_1 occurs and so on.
For any vector $\vec{x} \in E^{|\tau|}$ we denote by x_i its i-th coordinate and by $J_{\vec{x}}$ its support $\{i \in I_0 : x_i \neq 0\}$. We define as norm of $\vec{x}$ with respect to φ the vector $\mathrm{Nm}_\varphi(\vec{x}) := \prod\limits_{i=0}^{f-1} \varphi^i(\vec{x})$ and we write $\mathrm{v}_p(\mathrm{Nm}_\varphi(\vec{x})) := \mathrm{v}_p\left(\prod\limits_{i=0}^{f-1} x_i\right)$, where v_p is the normalized p-adic valuation of $\bar{\mathbb{Q}}_p$. If ℓ is an integer we write $\vec{\ell} = (\ell, \ell, ..., \ell)$ and $\mathrm{v}_p(\vec{x}) > \vec{\ell}$ (resp. if $\mathrm{v}_p(\vec{x}) \geq \vec{\ell}$) if and only if $\mathrm{v}_p(x_i) > \ell$ (resp. $v_p(x_i) \geq \ell$) for all i. Finally, for any matrix $A \in M_n(E^{|\tau|})$ we define as its φ-norm the matrix $\mathrm{Nm}_\varphi(A) := A\varphi(A) \cdots \varphi^{f-1}(A)$, with φ acting on each entry of A.

In §3 we construct the effective crystalline characters of G_{K_f}. More precisely, for $i = 0, 1, ..., f-1$ we construct E-characters χ_i of G_{K_f} with labeled Hodge-Tate weights $-e_{i+1} = (0, ..., -1, ...0)$ with the -1 appearing in the $(i+1)$-place for all i, and we show that any crystalline E-character of G_{K_f} with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$ can be written uniquely in the form $\chi = \eta \cdot \chi_0^{k_1} \cdot \chi_1^{k_2} \cdot \cdots \cdot \chi_{f-2}^{k_{f-1}} \cdot \chi_{f-1}^{k_0}$ for some unramified character η of G_{K_f}. In the same section we prove the following.

Theorem 1.3. *Let* $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$, *where the* k_i, $i = 0, 1, ..., f-1$ *are nonnegative integers. Let* f^+ *be the number of strictly positive* k_i *and assume that* $f^+ \geq 1$.

(i) The crystalline character $\chi_{\vec{\ell}} = \chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}$ *of* $G_{K_{2f}}$ *has labeled Hodge-Tate weights* $(-\ell_0, -\ell_1, ..., -\ell_{2f-1})$ *and does not extend to* G_{K_f}. *The induced representation* $\mathrm{Ind}_{K_{2f}}^{K_f}(\chi_{\vec{\ell}})$ *is irreducible and crystalline with labeled Hodge-Tate weights* $\{0, -k_i\}_{\tau_i}$.

(ii) Let V *be an irreducible two-dimensional crystalline* E*-representation of* G_{K_f} *with labeled Hodge-Tate weights* $\{0, -k_i\}_{\tau_i}$, *whose restriction to* $G_{K_{2f}}$ *is reducible. There exist an unramified character* η *of* G_{K_f} *and nonnegative integers* m_i, $i = 0, 1, ..., 2f-1$, *with* $\{m_i, m_{i+f}\} = \{0, k_i\}$ *for all* $i = 0, 1, ..., f-1$, *such that*

$$V \simeq \eta \otimes \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_0^{m_1} \cdot \chi_1^{m_2} \cdot \cdots \cdot \chi_{2f-2}^{m_{2f-1}} \cdot \chi_{2f-1}^{m_0}\right).$$

(iii) $\mathrm{Ind}_{K_{2f}}^{K_f}(\chi_{\vec{\ell}}) \simeq \mathrm{Ind}_{K_{2f}}^{K_f}(\chi_{\vec{m}})$ *if and only if* $\chi_{\vec{\ell}} = \chi_{\vec{m}}$ *or* $\chi_{\vec{\ell}}^{\sigma} = \chi_{\vec{m}}$, *where* $\chi_{\vec{\ell}}^{\sigma} = \chi_0^{\ell'_1} \cdot \chi_1^{\ell'_2} \cdots \chi_{2f-2}^{\ell'_{2f-1}} \cdot \chi_{2f-1}^{\ell'_f}$, *with* $\ell'_i = \ell_{i+f}$ *and indices viewed modulo* $2f$.

(iv) Up to twist by some unramified character, there exist precisely 2^{f^+-1} *distinct isomorphism classes of irreducible two-dimensional crystalline* E*-representations of* G_{K_f} *with labeled Hodge-Tate weights* $\{0, -k_i\}_{\tau_i}$, *induced from crystalline characters of* $G_{K_{2f}}$.

Next, we turn our attention to generically irreducible families of two-dimensional crystalline E-representations of G_{K_f}. For any irreducible effective two-dimensional crystalline E-representation of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$ which is induced from a crystalline character of $G_{K_{2f}}$, we construct an infinite family of crystalline E-representations of G_{K_f} of the same Hodge-Tate type which contains it. The members of each of these families have the same semisimplified mod p reductions which we explicitly compute.

Let $V_{\vec{\ell}} = \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}\right)$, where $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$ for all $i = 0, 1, ..., f-1$, and assume that at least one k_i is strictly positive. Theorem 1.3 asserts that $V_{\vec{\ell}}$ is irreducible and crystalline with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$. We describe the members of the family containing $V_{\vec{\ell}}$ in terms of their corresponding by the Colmez-Fontaine theorem weakly admissible filtered φ-modules.

Definition 1.4. *We define the following four types of matrices*

$$t_1\colon \begin{pmatrix} p^{k_i} & 0 \\ X_i & 1 \end{pmatrix},\ t_2\colon \begin{pmatrix} X_i & 1 \\ p^{k_i} & 0 \end{pmatrix},\ t_3\colon \begin{pmatrix} 1 & X_i \\ 0 & p^{k_i} \end{pmatrix},\ t_4 : \begin{pmatrix} 0 & p^{k_i} \\ 1 & X_i \end{pmatrix},$$

where the X_i *are indeterminates. Let* $k = \max\{k_i,\ i = 0, 1, ..., f-1\}$ *and let*

$$m := \begin{cases} \lfloor \frac{k-1}{p-1} \rfloor & \text{if } k \geq p \textit{ and } k_i \neq p \textit{ for some } i, \\ 0 & \text{if } k \leq p-1 \textit{ or } k_i = p \textit{ for all } i. \end{cases}$$

Let $P(\overrightarrow{X}) = (P_1(X_1), P_2(X_2), ..., P_f(X_f))$ *be a matrix whose coordinates* $P_j(X_j)$ *are matrices of type* 1, 2, 3 *or* 4. *To each such* f*-tuple we attach a type-vector* $\vec{i} \in \{1, 2, 3, 4\}^f$, *where for any* $j = 1, 2, ..., f$, *the* j*-th coordinate of* $\vec{i}$ *is defined to be the type of the matrix* P_j. *We write* $P(\overrightarrow{X}) = P^{\vec{i}}(\overrightarrow{X})$. *The set of all* f*-tuples of matrices of type* 1, 2, 3, 4 *will be denoted by* $\mathcal{P}$. *There is no loss to assume that the first* $f-1$ *coordinates of* $P(\overrightarrow{X})$ *are of type* 1 *or* 2 *(see Remark 6.13) and unless otherwise stated we always assume so. Matrices of type* t_1 *or* t_3 *are called of odd type while matrices of type* t_2 *or* t_4 *are called of even type.*

For any vector $\vec{a} = (\alpha_1, \alpha_2, ..., \alpha_f) \in (p^m \mathfrak{m}_E)^f$ we obtain a matrix

$$P^{\vec{i}}(\vec{\alpha}) = (P_1(\alpha_1), P_2(\alpha_2), ..., P_f(\alpha_f))$$

by evaluating each indeterminate X_i at α_i. We view indices of f-tuples mod f, so $P_f = P_0$. To construct the family containing $V_{\vec{\ell}}$ we choose the types of the matrices P_i as follows:
(1) If $\ell_1 = 0$, $P_1 = t_2$;
(2) If $\ell_1 = k_1 > 0$, $P_1 = t_1$.
For $i = 2, 3, ..., f-1$ we choose the type of the matrix P_i as follows:
(1) If $\ell_i = 0$, then:

- If an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, $P_i = t_2$;
- If an odd number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, $P_i = t_1$.

(2) If $\ell_i = k_i > 0$, then:

- If an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, $P_i = t_1$;
- If an odd number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, $P_i = t_2$.

Finally, we choose the type of the matrix P_0 as follows:
(1) If $\ell_0 = 0$, then:

- If an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_4$;

- If an odd number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_3$.

(2) If $\ell_0 = k_i > 0$, then:

- If an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_2$;
- If an odd number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_1$.

We define families of rank two filtered φ-modules $\left(\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{\alpha}), \varphi\right)$ over $E^{|\tau|}$ by equipping $\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{\alpha}) = E^{|\tau|}\eta_1 \bigoplus E^{|\tau|}\eta_2$ with the Frobenius endomorphism defined by $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2)\, P^{\vec{i}}(\vec{\alpha})$ and the filtration

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{\alpha})) = \begin{cases} E^{|\tau|}\eta_1 \bigoplus E^{|\tau|}\eta_2 & \text{if } \ j \leq 0, \\ E^{|\tau_{I_0}|}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } \ 1 \leq j \leq w_0, \\ E^{|\tau_{I_1}|}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } \ 1 + w_0 \leq j \leq w_1, \\ \cdots\cdots & \\ E^{|\tau_{I_{t-1}}|}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } \ 1 + w_{t-2} \leq j \leq w_{t-1}, \\ 0 & \text{if } \ j \geq 1 + w_{t-1}, \end{cases} \tag{1.1}$$

where $\vec{x} = (x_0, x_1, ..., x_{f-1})$ and $\vec{y} = (y_0, y_1, ..., y_{f-1})$, with

$$(x_i, y_i) = \begin{cases} (1, -\alpha_i) \text{ if } P_i \text{ has type 1 or 2,} \\ (-\alpha_i, 1) \text{ if } P_i \text{ has type 3 or 4.} \end{cases} \tag{1.2}$$

Theorem 1.5. *Let $\vec{i}$ be the type-vector attached to the f-tuple $(P_1, P_2, ..., P_f)$ defined above. For any $\vec{\alpha} \in (p^m \mathfrak{m}_E)^f$,*

(i) The filtered φ-module $\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{\alpha})$ is weakly admissible and corresponds to a two-dimensional crystalline E-representations $V_{\vec{k}}^{\vec{i}}(\vec{\alpha})$ of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$;

(ii) $V_{\vec{k}}^{\vec{i}}(\vec{0}) = \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}\right)$;

(iii) $\overline{V}_{\vec{k}}^{\vec{i}}(\vec{\alpha}) = \overline{V}_{\vec{k}}^{\vec{i}}(\vec{0})$;

(iv) $\left(\overline{V}_{\vec{k}}^{\vec{i}}(\vec{\alpha})_{|I_{K_f}}\right)^{s.s.} = \omega_{2f,\bar{\tau}_0}^{\beta} \bigoplus \omega_{2f,\bar{\tau}_0}^{p^f\beta}$, *where* $\beta = -\sum_{i=0}^{2f-1} p^i \ell_i$;

(v) The residual representation $\overline{V}_{\vec{k}}^{\vec{i}}(\vec{\alpha})$ is irreducible if and only if $1 + p^f \nmid \beta$;

(vi) Any irreducible member of the family $\left\{V_{\vec{k}}^{\vec{i}}(\vec{\alpha}),\ \vec{\alpha} \in (p^m\mathfrak{m}_E)^f\right\}$, other than $V_{\vec{k}}^{\vec{i}}(\vec{0})$, is non-induced.

Notice that in the cases where $1+p^f \nmid \beta$, all the members of the family $\left\{V_{\vec{k}}^{\vec{i}}(\vec{\alpha}),\ \vec{\alpha}\in(p^m\mathfrak{m}_E)^f\right\}$ are forced to be irreducible. Next, we compute the semisimplified reduction of any reducible two-dimensional crystalline E-representation of G_{K_f}. After enlarging E if necessary, any reducible rank two weakly admissible filtered φ-module $\mathbb{D}$ over $E^{|\tau|}$ with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$ contains an ordered basis $\underline{\eta}=(\eta_1,\eta_2)$ in which the matrix of Frobenius takes the form $\mathrm{Mat}_{\underline{\eta}}(\varphi)=\begin{pmatrix}\vec{\alpha} & \vec{0}\\ \vec{*} & \vec{\delta}\end{pmatrix}$ such that $\mathbb{D}_2=\left(E^{|\tau|}\right)\eta_2$ is a φ-stable weakly admissible submodule (see Proposition 6.4). The filtration of $\mathbb{D}$ in such a basis $\underline{\eta}$ has the form

$$\mathrm{Fil^j}(\mathbb{D})=\begin{cases} E^{|\tau|}\eta_1\bigoplus E^{|\tau|}\eta_2 & \text{if } j\le 0,\\ E^{|\tau_{I_0}|}(\vec{x}\eta_1+\vec{y}\eta_2) & \text{if } 1\le j\le w_0,\\ E^{|\tau_{I_1}|}(\vec{x}\eta_1+\vec{y}\eta_2) & \text{if } 1+w_0\le j\le w_1,\\ \quad\cdots\cdots & \\ E^{|\tau_{I_{t-1}}|}(\vec{x}\eta_1+\vec{y}\eta_2) & \text{if } 1+w_{t-2}\le j\le w_{t-1},\\ 0 & \text{if } j\ge 1+w_{t-1},\end{cases}$$

for some vectors $\vec{x},\vec{y}\in E^{|\tau|}$ with $(x_i,y_i)\neq(0,0)$ for all i. For each $i\in I_0$, let

$$m_i=\begin{cases}0 & \text{if } x_i\neq 0\ ,\\ k_i & \text{if } x_i=0.\end{cases}$$

Theorem 1.6. *Let V be any reducible two-dimensional crystalline E-representation of G_{K_f} with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$ corresponding to the weakly admissible filtered φ-module $\mathbb{D}$ as above.*

(i) There exist unramified characters η_i of G_{K_f} such that

$$V\simeq\begin{pmatrix}\psi_1 & *\\ 0 & \psi_2\end{pmatrix},$$

where $\psi_1=\eta_1\cdot\chi_0^{m_1}\cdot\cdots\cdot\chi_{f-2}^{m_{f-1}}\cdot\chi_{f-1}^{m_0}$ and $\psi_2=\eta_2\cdot\chi_0^{k_1-m_1}\cdot\chi_1^{k_2-m_2}\cdot\cdots\cdot\chi_{f-2}^{k_{f-1}-m_{f-1}}\cdot\chi_{f-1}^{k_0-m_0}$;

(ii) $\left(\overline{V}_{|I_K}\right)^{s.s.}=\omega_{f,\bar{\tau}_0}^{\beta_1}\bigoplus\omega_{f,\bar{\tau}_0}^{\beta_2}$, where $\beta_1=-\sum_{i=0}^{f-1}m_ip^i$ and $\beta_2=\sum_{i=0}^{f-1}(m_i-k_i)\,p^i$.

The computation of the semisimplified mod p reduction of a reducible two-dimensional crystalline representation is easy and does not require the construction of the Wach module (see §2.1 for the definition) corresponding to some G_{K_f}-stable lattice contained in it. Computing the non-semisimplified mod p reduction of a two-dimensional crystalline representations with reducible

reduction is an interesting problem not pursued in this paper. For results of this flavour for $K = \mathbb{Q}_{p^2}$, see [CD09].
Up to twist by some unramified character, any split-reducible two-dimensional crystalline E-representations of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$ is of the form

$$V_{\vec{\ell},\vec{\ell}'}(\eta) = \eta \cdot \chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \dots \cdot \chi_{f-2}^{\ell_{f-1}} \cdot \chi_{f-1}^{\ell_0} \bigoplus \chi_0^{\ell_1'} \cdot \chi_1^{\ell_2'} \cdot \dots \cdot \chi_{f-2}^{\ell_{f-1}'} \cdot \chi_{f-1}^{\ell_0'},$$

for some unramified character η and some nonnegative integers ℓ_i and ℓ_i' such that $\{\ell_i, \ell_i'\} = \{0, k_i\}$ for all i. In Theorem 1.5 we showed that each irreducible representation of G_{K_f} induced from some crystalline character of $G_{K_{2f}}$ belongs to an infinite family of crystalline representations of the same Hodge-Tate types with the same mod p reductions. In the next theorem we prove the same for any split-reducible, non-ordinary two-dimensional crystalline E-representation of G_{K_f}. We list the weakly admissible filtered φ-modules corresponding to these families. In order to construct the infinite family containing $V_{\vec{\ell},\vec{\ell}'}(\eta)$, we define a matrix $P^{\vec{i}}(\overrightarrow{X}) \in \mathcal{P}$ by choosing the $(f-1)$-tuple $(P_1, P_2, ..., P_{f-1})$ as in Theorem 1.5. If $\eta = \eta_c$ is the unramified character which maps the geometric Frobenius Frob_{K_f} of G_{K_f} to c, we replace the entry p^{k_0} in the definition of the matrix P_0 by cp^{k_0}. The type of the matrix P_0 is chosen as follows:
(1) If $\ell_0 = 0$, then:

- If an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_3$;
- If an odd number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_4$.

(2) If $\ell_0 = k_0 > 0$, then:

- If an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_1$;
- If an odd number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, $P_0 = t_2$.

Using the matrices $P^{\vec{i}}(\overrightarrow{X})$ we define families of two-dimensional crystalline E-representations $\left\{V_{\vec{k}}^{\vec{i}}(\vec{\alpha}),\ \vec{\alpha} \in (p^m \mathfrak{m}_E)^f\right\}$ of G_{K_f} as in Theorem 1.5 and prove the following.

Theorem 1.7. *Let $\vec{i}$ be the type-vector attached to the f-tuple $(P_1, P_2, ..., P_f)$ defined above.*

(i) There exists some unramified character μ such that $V_{\vec{k}}^{\vec{i}}(\vec{0}) \simeq \mu \otimes V_{\vec{\ell},\vec{\ell}'}(\eta)$;

(ii) Assume that $\vec{\ell} \neq \vec{0}$ and $\vec{\ell}' \neq \vec{0}$. For any $\vec{\alpha} \in (p^m \mathfrak{m}_E)^f$, $\overline{V}_{\vec{k}}^{\vec{i}}(\vec{\alpha}) \simeq \overline{V}_{\vec{k}}^{\vec{i}}(\vec{0})$;

(iii) $\overline{V}_{\vec{\ell},\vec{\ell}'}(\eta)_{|I_{K_f}} = \omega^{\beta}_{f,\bar{\tau}_0} \bigoplus \omega^{\beta'}_{f,\bar{\tau}_0}$, *where* $\beta = -\sum_{i=0}^{f-1} \ell_i p^i$ *and* $\beta' = -\sum_{i=0}^{f-1} \ell'_i p^i$.

A family as in Theorem 1.7 can contain simultaneously split and non-split reducible, as well as irreducible crystalline representations. For example, in the family $\left\{V^{(1,3)}_{\vec{k}}(\vec{\alpha}),\ \vec{\alpha} \in (p^m \mathfrak{m}_E)^2\right\}$, the representation $V^{(1,3)}_{\vec{k}}(\vec{\alpha})$ is split-reducible if and only if $\vec{\alpha} = \vec{0}$, non-split-reducible if and only if precisely one of the coordinates α_i of $\vec{\alpha}$ is zero, and irreducible if and only if $\alpha_0\alpha_1 \neq 0$ (cf. Proposition 6.21). The families of Wach modules which give rise to $V^{(1,3)}_{\vec{k}}(\vec{\alpha})$ contain infinite sub-families of non-split reducible Wach modules which can be used to compute the non-semisimplified mod p reduction of the corresponding crystalline representations with respect to G_{K_f}-stable $\mathcal{O}_E$-lattices. Some reducible two-dimensional crystalline representations with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$ are easily recognized by looking at their trace of Frobenius. More precisely, if $\mathrm{Tr}\left(\varphi^f\right) \in \mathcal{O}_E^{\times}$, then the representation is reducible (cf. Proposition 6.5), with the converse being false.

2 Overview of the theory

2.1 Étale (φ, Γ)-modules and Wach modules

The general theory of (φ, Γ)-modules works for arbitrary finite extensions K of $\mathbb{Q}_p$. However, a theory of Wach modules, which is our main tool and which we briefly recall in this section, currently exists only when K is unramified over $\mathbb{Q}_p$. We temporarily allow K to be any finite extension of $\mathbb{Q}_p$; we will go back to assume that K is unramified after Theorem 2.2. Let $K_n = K(\zeta_{p^n})$, where ζ_{p^n} is a primitive p^n-th root of unity inside $\bar{\mathbb{Q}}_p$, and let $K_\infty = \cup_{n \geq 1} K_n$. Let $\chi : G_K \to \mathbb{Z}_p^{\times}$ be the cyclotomic character, and let $H_K = \ker \chi = \mathrm{Gal}(\bar{\mathbb{Q}}_p/K_\infty)$ and $\Gamma_K = G_K/H_K = \mathrm{Gal}(K_\infty/K)$. Fontaine ([Fon90]) has constructed topological rings $\mathbb{A}$ and $\mathbb{B}$ endowed with continuous commuting Frobenius φ and $G_{\mathbb{Q}_p}$-actions. Unless otherwise stated and whenever applicable, continuity means continuity with respect to the topologies induced by the weak topologies of the rings $\mathbb{A}$ and $\mathbb{B}$. Let $\mathbb{A}_K = \mathbb{A}^{H_K}$ and $\mathbb{B}_K = \mathbb{B}^{H_K}$, and define $\mathbb{A}_{K,E} := \mathcal{O}_E \otimes_{\mathbb{Z}_p} \mathbb{A}_K$ and $\mathbb{B}_{K,E} := E \otimes_{\mathbb{Q}_p} \mathbb{B}_K$. The actions of φ and Γ_K extend to $\mathbb{A}_{K,E}$ and $\mathbb{B}_{K,E}$ by $\mathcal{O}_E$ (resp. E, k_E)-linearity, and one easily sees that $\mathbb{A}_{K,E} = \mathbb{A}_E^{H_K}$ and $\mathbb{B}_{K,E} = \mathbb{B}_E^{H_K}$.

Definition 2.1. *A* (φ, Γ)*-module over* $\mathbb{A}_{K,E}$ *(resp.* $\mathbb{B}_{K,E}$*) is an* $\mathbb{A}_{K,E}$*-module of finite type (resp. a free* $\mathbb{B}_{K,E}$*-module of finite type) endowed with a semilinear and continuous action of* Γ_K*, and with a semilinear map* φ *which commutes with the action of* Γ_K*. A* (φ, Γ)*-module* M *over* $\mathbb{A}_{K,E}$ *is called étale if* $\varphi^*(M) = M$*, where* $\varphi^*(M)$ *is the* $\mathbb{A}_{K,E}$*-module generated by the set* $\varphi(M)$*. A* (φ, Γ)*-module* M *over* $\mathbb{B}_{K,E}$ *is called étale if it contains a basis* $(e_1, ..., e_d)$ *over* $\mathbb{B}_{K,E}$ *such that* $(\varphi(e_1), ..., \varphi(e_d)) = (e_1, ..., e_d)A$ *for some matrix* $A \in \mathrm{GL}_d(\mathbb{A}_{K,E})$.

If V is a continuous E-linear representation of G_K, we equip the $\mathbb{B}_{K,E}$-module $\mathbb{D}(V) := (\mathbb{B}_E \otimes_E V)^{H_K}$ with a Frobenius endomorphism φ defined by $\varphi(b \otimes v) := \varphi(b) \otimes v$, where φ on the right hand side is the Frobenius of $\mathbb{B}_E$, and with an action of Γ_K given by $\bar{g}(b \otimes v) := gb \otimes gv$ for any $g \in G_K$. This Γ_K-action commutes with φ and is continuous. Moreover, $\mathbb{D}(V)$ is an étale (φ, Γ)-module over $\mathbb{B}_{K,E}$. Conversely, if D is an étale (φ, Γ)-module over $\mathbb{B}_{K,E}$, let $\mathbb{V}(D) := \left(\mathbb{B}_E \otimes_{\mathbb{B}_{K,E}} D\right)^{\varphi=1}$, where $\varphi(b \otimes d) := \varphi(b) \otimes \varphi(d)$. The E-vector space $\mathbb{V}(D)$ is finite dimensional and is equipped with a continuous E-linear G_K-action given by $g(b \otimes d) := gb \otimes \bar{g}d$. We have the following fundamental theorem of Fontaine.

Theorem 2.2. *[Fon90]*

(i) There is an equivalence of categories between continuous E-linear representations of G_K and étale (φ, Γ)-modules over $\mathbb{B}_{K,E}$ given by

$$\mathbb{D} : \mathrm{Rep}_E(G_K) \to \mathcal{M}od^{\acute{e}t}_{(\varphi,\Gamma)}(\mathbb{B}_{K,E}) : V \longmapsto \mathbb{D}(V) := (\mathbb{B}_E \otimes_E V)^{H_K},$$

with quasi-inverse functor

$$\mathbb{V} : \mathcal{M}od^{\acute{e}t}_{(\varphi,\Gamma)}(\mathbb{B}_{K,E}) \to \mathrm{Rep}_E(G_K) : D \longmapsto \mathbb{V}(D) := \left(\mathbb{B}_E \otimes_{\mathbb{B}_{K,E}} D\right)^{\varphi=1}.$$

(ii) There is an equivalence of categories between continuous $\mathcal{O}_E$-linear representations of G_K and étale (φ, Γ)-modules over $\mathbb{A}_{K,E}$ given by

$$\mathbb{D} : \mathrm{Rep}_{\mathcal{O}_E}(G_K) \to \mathcal{M}od^{\acute{e}t}_{(\varphi,\Gamma)}(\mathbb{A}_{K,E}) : \mathrm{T} \longmapsto \mathbb{D}(T) := (\mathbb{A}_E \otimes_{\mathcal{O}_E} \mathrm{T})^{H_K},$$

with quasi-inverse functor

$$\mathbb{T} : \mathcal{M}od^{\acute{e}t}_{(\varphi,\Gamma)}(\mathbb{A}_{K,E}) \to \mathrm{Rep}_{\mathcal{O}_E}(G_K) : D \longmapsto \mathbb{T}(D) := \left(\mathbb{A}_E \otimes_{\mathbb{A}_{K,E}} D\right)^{\varphi=1}.$$

We return to assume that K is unramified over $\mathbb{Q}_p$. In this case $\mathbb{A}_K$ has the form $\mathbb{A}_K = \{\sum_{n=-\infty}^{\infty} \alpha_n \pi_K^n : \alpha_n \in \mathcal{O}_K \text{ and } \lim_{n\to-\infty} \alpha_n = 0\}$ for some element π_K which can be thought of as a formal variable. The Frobenius endomorphism φ of $\mathbb{A}_K$ extends the absolute Frobenius of $\mathcal{O}_K$ and is such that $\varphi(\pi_K) = (1+\pi_K)^p - 1$. The Γ_K-action of $\mathbb{A}_K$ is $\mathcal{O}_K$-linear, commutes with Frobenius, and is such that $\gamma(\pi_K) = (1+\pi_K)^{\chi(\gamma)} - 1$ for all $\gamma \in \Gamma_K$. For simplicity we write π instead of π_K. The ring $\mathbb{A}_K$ is local with maximal ideal (p), fraction field $\mathbb{B}_K = \mathbb{A}_K[\frac{1}{p}]$, and residue field $\mathbb{E}_K := k_K((\pi))$, where k_K is the residue field of K. The rings $\mathbb{A}_K$, $\mathbb{A}_{K,E}$, $\mathbb{B}_K$ and $\mathbb{B}_{K,E}$ contain the subrings $\mathbb{A}_K^+ = \mathcal{O}_K[[\pi]]$, $\mathbb{A}_{K,E}^+ := \mathcal{O}_E \otimes_{\mathbb{Z}_p} \mathbb{A}_K^+$, $\mathbb{B}_K^+ = \mathbb{A}_K^+[\frac{1}{p}]$ and $\mathbb{B}_{K,E}^+ := E \otimes_{\mathbb{Q}_p} \mathbb{B}_K^+$ respectively, and these subrings are equipped with the restrictions of the φ and the Γ_K-actions of the rings containing them. There is a ring isomorphism

$$\xi : \mathbb{A}_{K,E}^+ \to \prod_{\tau : K \hookrightarrow E} \mathcal{O}_E[[\pi]] \tag{2.1}$$

given by $\xi(a\otimes b) = (a\tau_0(b), a\tau_1(b), ..., a\tau_{f-1}(b))$, where $\tau_i\left(\sum_{n=0}^{\infty}\beta_n\pi^n\right) = \sum_{n=0}^{\infty}\tau_i(\beta_n)\pi^n$ for all $b=\sum_{n=0}^{\infty}\beta_n\pi^n\in\mathbb{A}_K^+$. The ring $\mathcal{O}_E[[\pi]]^{|\tau|} := \prod_{\tau:K\hookrightarrow E}\mathcal{O}_E[[\pi]]$ is equipped via ξ with commuting $\mathcal{O}_E$-linear actions of φ and Γ_K given by

$$\varphi(\alpha_0(\pi),\alpha_1(\pi),...,\alpha_{f-1}(\pi)) = (\alpha_1(\varphi(\pi)),...,\alpha_{f-1}(\varphi(\pi)),\alpha_0(\varphi(\pi))) \tag{2.2}$$

$$\text{and } \gamma(\alpha_0(\pi),\alpha_1(\pi),...,\alpha_{f-1}(\pi)) = (\alpha_0(\gamma\pi),\alpha_1(\gamma\pi),...,\alpha_{f-1}(\gamma\pi)) \tag{2.3}$$

for all $\gamma\in\Gamma_K$.

Definition 2.3. *Suppose $k\geq 0$. A Wach module over $\mathbb{A}_{K,E}^+$ (resp. $\mathbb{B}_{K,E}^+$) with weights in $[-k;\ 0]$ is a free $\mathbb{A}_{K,E}^+$-module (resp. $\mathbb{B}_{K,E}^+$-module) N of finite rank, endowed with an action of Γ_K which becomes trivial modulo π, and also with a Frobenius map φ which commutes with the action of Γ_K and such that $\varphi(N)\subset N$ and $N/\varphi^*(N)$ is killed by q^k, where $q:=\varphi(\pi)/\pi$.*

A natural question is to determine the types of étale (φ,Γ)-modules which correspond to crystalline representations via Fontaine's functor. An answer is given by the following theorem of Berger who built on previous work of Wach [Wac96], [Wac97] and Colmez [Col99].

Theorem 2.4. *[Ber04a]*

(i) An E-linear representation V of G_K is crystalline with Hodge-Tate weights in $[-k;\ 0]$ if and only if $\mathbb{D}(V)$ contains a unique Wach module $\mathbb{N}(V)$ of rank $\dim_E V$ with weights in $[-k;\ 0]$. The functor $V\mapsto\mathbb{N}(V)$ defines an equivalence of categories between crystalline representations of G_K and Wach modules over $\mathbb{B}_{K,E}^+$, compatible with tensor products, duality and exact sequences.

(ii) For a given crystalline E-representation V, the map $\mathrm{T}\mapsto\mathbb{N}(\mathrm{T}):=\mathbb{N}(V)\cap\mathbb{D}(\mathrm{T})$ induces a bijection between G_K-stable, $\mathcal{O}_E$-lattices of V and Wach modules over $\mathbb{A}_{K,E}^+$ which are $\mathbb{A}_{K,E}^+$-lattices contained in $\mathbb{N}(V)$. Moreover $\mathbb{D}(\mathrm{T})=\mathbb{A}_{K,E}\otimes_{\mathbb{A}_{K,E}^+}\mathbb{N}(\mathrm{T})$.

(iii) If V is a crystalline E-representation of G_K, and if we endow $\mathbb{N}(V)$ with the filtration $\mathrm{Fil}^{\mathrm{i}}\mathbb{N}(V)=\{x\in\mathbb{N}(V)|\varphi(x)\in q^i\mathbb{N}(V)\}$, then we have an isomorphism

$$\mathbb{D}_{\mathrm{cris}}(V)\to\mathbb{N}(V)/\pi\mathbb{N}(V)$$

of filtered φ-modules over $E^{|\tau|}$ (with the induced filtration on $\mathbb{N}(V)/\pi\mathbb{N}(V)$).

In view of Theorems 2.2 and 2.4, constructing the Wach module $\mathbb{N}(T)$ of a G_K-stable $\mathcal{O}_E$-lattice T in a crystalline representation V amounts to explicitly constructing the crystalline representation. Indeed, we have

$$V\simeq E\otimes_{\mathcal{O}_E}\left(\mathbb{A}_{K,E}\otimes_{\mathbb{A}_{K,E}^+}\mathbb{N}(\mathrm{T})\right)^{\varphi=1}.$$

An obvious advantage of using Wach modules is that instead of working with the more complicated rings $\mathbb{A}_{K,E}$ and $\mathbb{B}_{K,E}$, one works with the simpler ones $\mathbb{A}^+_{K,E}$ and $\mathbb{B}^+_{K,E}$.

2.2 Wach modules of restricted representations

In this section we relate the Wach module of an effective n-dimensional effective crystalline E-representation V_{K_f} of G_{K_f} to the Wach module of its restriction $V_{K_{df}}$ to $G_{K_{df}}$.

Proposition 2.5. *(i) The Wach module associated to the representation $V_{K_{df}}$ is given by*

$$\mathbb{N}(V_{K_{df}}) = \mathbb{B}^+_{K_{df},E} \otimes_{\mathbb{B}^+_{K_f,E}} \mathbb{N}(V_{K_f}),$$

where $\mathbb{N}(V_{K_f})$ is the Wach module associated to V_{K_f}.

(ii) If T_{K_f} is a G_{K_f}-stable $\mathcal{O}_E$-lattice in V_f associated to the Wach-module $\mathbb{N}(\mathrm{T}_{K_f})$, then V_{df} contains some $G_{K_{df}}$-stable $\mathcal{O}_E$-lattice $\mathrm{T}_{K_{df}}$ whose associated Wach module is

$$\mathbb{N}(\mathrm{T}_{K_{df}}) = \mathbb{A}^+_{K_{df},E} \otimes_{\mathbb{A}^+_{K_f,E}} \mathbb{N}(\mathrm{T}_{K_f}).$$

Proof. (i) Since $\mathbb{N}(V_{K_f})$ is a free $\mathbb{B}^+_{K_f,E}$-module of rank $\dim_E V$ contained in $\mathbb{D}(V_{K_f})$, $N := \mathbb{B}^+_{K_{df},E} \otimes_{\mathbb{B}^+_{K_f,E}} \mathbb{N}(V_{K_f})$ is a free $\mathbb{B}^+_{K_{df},E}$-module of rank $\dim_E V$ contained in $\mathbb{D}(V_{K_{df}}) \supseteq \mathbb{D}(V_{K_f})$. Moreover, N is endowed with an action of $\Gamma_{K_{df}}$ which becomes trivial modulo π, and also with a Frobenius map φ which commutes with the action of $\Gamma_{K_{df}}$ and such that $\varphi(N) \subset N$ and $N/\varphi^*(N)$ is killed by q^k. Hence $N = \mathbb{N}(V_{K_{df}})$ by the uniqueness part of Theorem 2.4(i). Part (ii) follows immediately from Theorem 2.4(ii) since $\mathbb{A}^+_{K_{df},E} \otimes_{\mathbb{A}^+_{K_f,E}} \mathbb{N}(\mathrm{T}_{K_f})$ is an $\mathbb{A}^+_{K_{df},E}$-lattice in $\mathbb{N}(V_{K_{df}})$. ∎

We fix once and for all an embedding $\tau^0_{K_{df}} : K_{df} \hookrightarrow E$ and we let $\tau^j_{K_{df}} = \tau^0_{K_{df}} \circ \sigma^j_{K_{df}}$ for $j = 0, 1, ..., df-1$, where $\sigma_{K_{df}}$ is the absolute Frobenius of K_{df}. We fix the df-tuple of embeddings $\mid \tau_{K_{df}} \mid := (\tau^0_{K_{df}}, \tau^1_{K_{df}}, ..., \tau^{df-1}_{K_{df}})$. We adjust the notation of §1.1 for the embeddings of K_f into E to the relative situation considered in this section. Let ι be the natural inclusion of K_f into K_{df}, in the sense that $\iota \circ \sigma_{K_f} = \sigma_{K_{df}} \circ \iota$, where σ_{K_f} is the absolute Frobenius of K_f. This induces a natural inclusion of $\mathbb{A}^+_K$ to $\mathbb{A}^+_{K_{df}}$ which we also denote by ι. Let $\tau^j_{K_f} := \tau^0_{K_{df}} \circ \iota \circ \sigma^j_{K_f}$ for $j = 0, 1, ..., f-1$. We fix the f-tuple of embeddings $\mid \tau_{K_f} \mid := (\tau^0_{K_f}, \tau^1_{K_f}, ..., \tau^{f-1}_{K_f})$. Since the restriction of $\sigma_{K_{df}}$ to K_f is σ_{K_f}, we obtain the following commutative diagram

$$\begin{array}{ccc} \mathbb{A}^+_{K_f,E} & \xrightarrow{\xi_{\mathrm{K_f}}} & \mathcal{O}_E^{|\tau_{K_f}|}[[\pi]] \\ {\scriptstyle 1_{\mathcal{O}_{\mathrm{E}}}\otimes\iota}\big\downarrow & & \big\downarrow{\scriptstyle\theta} \\ \mathbb{A}^+_{K_{df},E} & \xrightarrow{\xi_{\mathrm{K_{df}}}} & \mathcal{O}_E^{|\tau_{K_{df}}|}[[\pi]] \end{array}$$

where θ is the ring homomorphism defined by

$$\begin{aligned}\theta(\alpha_0,\alpha_1,...,\alpha_{f-1}) &= \underbrace{(\alpha_0,\alpha_1,...,\alpha_{f-1},\alpha_0,\alpha_1,...,\alpha_{f-1},...,\alpha_0,\alpha_1,...,\alpha_{f-1})}_{d\text{-times}} \\ &=: (\alpha_0,\alpha_1,...,\alpha_{f-1})^{\otimes d}.\end{aligned}$$

For any matrix $A\in M_n\left(\mathcal{O}_E^{|\tau_{K_f}|}[[\pi]]\right)$ we denote by $A^{\otimes d}$ the matrix obtained by replacing each entry $\vec{\alpha}$ of A by $\vec{\alpha}^{\otimes d}$. A similar commutative diagram is obtained by replacing $\mathbb{A}^+_K$ by $\mathbb{B}^+_K$ and $\mathcal{O}_E^{|\tau_K|}[[\pi]]$ by $\mathcal{O}_E^{|\tau_K|}[[\pi]][\frac{1}{p}]$. The following proposition follows easily from the discussion above.

Proposition 2.6. *Let V_{K_f}, $V_{K_{df}}$, T_{K_f}, and $\mathrm{T}_{K_{df}}$ be as in Proposition 2.5.*

(i) If the Wach module $\mathbb{N}(V_{K_f})$ of V_{K_f} is defined by the actions of φ and Γ_{K_f} given by $(\varphi(\eta_1),\varphi(\eta_2),...,\varphi(\eta_n))=\underline{\eta}\cdot\Pi_{K_f}$ and $(\gamma(\eta_1),\gamma(\eta_2),...,\gamma(\eta_n))=\underline{\eta}\cdot G^{\gamma}_{K_f}$ for all $\gamma\in\Gamma_{K_f}$ for some ordered basis $\underline{\eta}=(\eta_1,\eta_2,...,\eta_n)$, then the Wach module $\mathbb{N}(V_{K_{df}})$ of $V_{K_{df}}$ is defined by $(\varphi(\eta'_1),\varphi(\eta'_2),...,\varphi(\eta'_n))=\underline{\eta}'\cdot\Pi_{K_{df}}$ and $(\gamma(\eta'_1),\gamma(\eta'_2),...,\gamma(\eta'_n))=\underline{\eta}'\cdot G^{\gamma}_{K_{df}}$ for all $\gamma\in\Gamma_{K_{df}}$, where $\Pi_{K_{df}}=(\Pi_{K_f})^{\otimes d}$ and $G^{\gamma}_{K_{df}}=\left(G^{\gamma}_{K_f}\right)^{\otimes d}$ for all $\gamma\in\Gamma_{K_{df}}$, for some ordered basis $\underline{\eta}'$ of $\mathbb{N}(V_{K_{df}})$.

(ii) If the Wach module $\mathbb{N}(\mathrm{T}_{K_f})$ of T_{K_f} is defined by the actions of φ and Γ_{K_f} given by $(\varphi(\eta_1),\varphi(\eta_2),...,\varphi(\eta_n))=\underline{\eta}\cdot\Pi_{K_f}$ and $(\gamma(\eta_1),\gamma(\eta_2),...,\gamma(\eta_n))=\underline{\eta}\cdot G^{\gamma}_{K_f}$ for all $\gamma\in\Gamma_{K_f}$ for some ordered basis $\underline{\eta}=(\eta_1,\eta_2,...,\eta_n)$, then the Wach module $\mathbb{N}(\mathrm{T}_{K_{df}})$ of $\mathrm{T}_{K_{df}}$ is defined by $(\varphi(\eta'_1),\varphi(\eta'_2),...,\varphi(\eta'_n))=\underline{\eta}'\cdot\Pi_{K_{df}}$ and $(\gamma(\eta'_1),\gamma(\eta'_2),...,\gamma(\eta'_n))=\underline{\eta}'\cdot G^{\gamma}_{K_{df}}$ for all $\gamma\in\Gamma_{K_{df}}$, where $\Pi_{K_{df}}=(\Pi_{K_f})^{\otimes d}$ and $G^{\gamma}_{K_{df}}=\left(G^{\gamma}_{K_f}\right)^{\otimes d}$ for all $\gamma\in\Gamma_{K_{df}}$, for some ordered basis $\underline{\eta}'$ of $\mathbb{N}(V_{K_{df}})$.

Corollary 2.7. *If V_{K_f} is a two-dimensional effective crystalline E-representation of G_{K_f} with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$, $i=0,1,...,f-1$, then $V_{K_{df}}$ is an effective crystalline E-representation of $G_{K_{df}}$ with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$, $i=0,1,...,df-1$, with $k_j=k_j$ for all $i,j=0,1,...,df-1$ with $i\equiv j \bmod f$.*

Proof. By Proposition 2.6 there exist ordered bases $\underline{\eta}$ and $\underline{\eta}'$ of $\mathbb{N}(V_{K_f})$ and $\mathbb{N}(V_{K_{df}})$ respectively, such that $\varphi\left(\underline{\eta}\right) = \underline{\eta} \cdot \Pi_{K_f}$, $\gamma\left(\underline{\eta}\right) = \underline{\eta} \cdot G^{\gamma}_{K_f}$ for all $\gamma \in \Gamma_{K_f}$ and $\varphi\left(\underline{\eta}'\right) = \underline{\eta}' \cdot \left(\Pi_{K_f}\right)^{\otimes d}$, $\gamma\left(\underline{\eta}'\right) = \underline{\eta}' \cdot \left(G^{\gamma}_{K_f}\right)^{\otimes d}$ for all $\gamma \in \Gamma_{K_{df}}$. By Theorem 2.4, $x \in \mathrm{Fil}^{\mathrm{j}}\left(\mathbb{N}(V_{K_f})\right)$ if and only if $\varphi\left(x\right) \in q^j\mathbb{N}(V_{K_f})$, from which it follows that $\mathrm{Fil}^{\mathrm{j}}\left(\mathbb{N}(V_{K_{df}})\right) = \left(\mathrm{Fil}^{\mathrm{j}}\left(\mathbb{N}(V_{K_f})\right)\right)^{\otimes d}$ for all j. By Theorem 2.4, $\mathbb{D}(V_{K_f}) \simeq \mathbb{N}(V_{K_f})/\pi\mathbb{N}(V_{K_f})$ as filtered φ-modules over $E^{|\tau_{K_f}|}$. This implies that $\mathrm{Fil}^{\mathrm{j}}\left(\mathbb{D}(V_{K_{df}})\right) = \left(\mathrm{Fil}^{\mathrm{j}}\left(\mathbb{D}(V_{K_f})\right)\right)^{\otimes d}$ for all j and the corollary follows. □

3 Effective Wach modules of rank one

In this section we construct the rank one Wach modules over $\mathcal{O}_E[[\pi]]^{|\tau|}$ with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$.

Definition 3.1. *Recall that* $q = \frac{\varphi(\pi)}{\pi}$ *where* $\varphi\left(\pi\right) = (1+\pi)^p - 1$. *We define* $q_1 = q$ *and* $q_n = \varphi^{n-1}\left(q\right)$ *for all* $n \geq 1$. *Let* $\lambda_f = \prod_{n=0}^{\infty}\left(\frac{q_{nf+1}}{p}\right)$. *For each* $\gamma \in \Gamma_K$, *we define* $\lambda_{f,\gamma} = \frac{\lambda_f}{\gamma\lambda_f}$.

Lemma 3.2. *For each* $\gamma \in \Gamma_K$, *the functions* λ_f *and* $\lambda_{f,\gamma} \in \mathbb{Q}_p[[\pi]]$ *have the following properties:*

(i) $\lambda_f(0) = 1$;

(ii) $\lambda_{f,\gamma} \in 1 + \pi\mathbb{Z}_p\left[[\pi]\right]$.

Proof. (i) This is clear since $\frac{q_n(0)}{p} = 1$ for all $n \geq 1$. (ii) One can easily check that $\frac{q}{\gamma q} \in 1 + \pi\mathbb{Z}_p\left[[\pi]\right]$. From this we deduce that $\lambda_{f,\gamma} \in 1 + \pi\mathbb{Z}_p\left[[\pi]\right]$. □

Consider the rank one module $\mathbb{N}_{\vec{k},c} = \left(\mathcal{O}_E[[\pi]]^{|\tau|}\right)\eta$ equipped with the semilinear φ and Γ_K-actions defined by $\varphi(\eta) = (c \cdot q^{k_1}, q^{k_2}, ..., q^{k_{f-1}}, q^{k_0})\eta$ and $\gamma(\eta)=(g_1^{\gamma}(\pi), g_2^{\gamma}(\pi), ...g_{f-1}^{\gamma}(\pi), g_0^{\gamma}(\pi))\eta$ for all $\gamma \in \Gamma_K$, where $c \in \mathcal{O}_E^{\times}$. We want to define the functions $g_i(\pi) = g_i^{\gamma}(\pi) \in \mathcal{O}_E[[\pi]]$ appropriately to make $\mathbb{N}_{\vec{k},c}$ a Wach module over $\mathcal{O}_E[[\pi]]^{|\tau|}$. The actions of φ and γ should commute and a short computation shows that g_0 should satisfy the equation

$$\varphi^f\left(g_0\right) = g_0\left(\frac{\gamma q}{q}\right)^{k_0}\varphi(\frac{\gamma q}{q})^{k_1}\cdots\varphi^{f-1}(\frac{\gamma q}{q})^{k_{f-1}}. \tag{3.1}$$

Lemma 3.3. *Equation 3.1 has a unique* $\equiv 1 \mathrm{mod}\ \pi$ *solution in* $\mathbb{Z}_p[[\pi]]$ *given by*

$$g_0 = \lambda_{f,\gamma}^{k_0}\varphi(\lambda_{f,\gamma})^{k_1}\varphi^2(\lambda_{f,\gamma})^{k_2}\cdots\varphi^{f-1}(\lambda_{f,\gamma})^{k_{f-1}}.$$

Proof. Notice that $\varphi^f(\lambda_f)=\frac{\lambda_f}{(\frac{q}{p})}$ and $\varphi^f(\gamma\lambda_f)=\frac{\gamma\lambda_f}{(\frac{\gamma q}{p})}$, hence $\lambda_{f,\gamma}=\frac{\lambda_f}{\gamma\lambda_f}$ solves the equation $\varphi^f(u)=u\left(\frac{\gamma q}{q}\right)$. It is straightforward to check that

$$g_0=\lambda_{f,\gamma}^{k_0}\varphi(\lambda_{f,\gamma})^{k_1}\varphi^2(\lambda_{f,\gamma})^{k_2}\cdots\varphi^{f-1}(\lambda_{f,\gamma})^{k_{f-1}}$$

is a solution of equation 3.1. By Lemma 3.2, $g_0\equiv 1 \bmod \pi$. If g_0 and g_0' are two solutions of equation 3.1 congruent to $1 \bmod \pi$, then $(\frac{g_0'}{g_0})\in\mathbb{Z}_p[[\pi]]$ is fixed by φ^f and is congruent to $1 \bmod \pi$, hence equals 1. □

Commutativity of φ with the Γ_K-actions implies that

$$g_1=(\frac{q}{\gamma q})^{k_1}\varphi(\frac{q}{\gamma q})^{k_2}\cdots\varphi^{f-2}(\frac{q}{\gamma q})^{k_{f-1}}\varphi^{f-1}(\lambda_{f,\gamma})^{k_0}\varphi^f(\lambda_{f,\gamma})^{k_1}\cdots\varphi^{2f-2}(\lambda_{f,\gamma})^{k_{f-1}},$$

$$\cdots\cdots$$

$$g_{f-2}=(\frac{q}{\gamma q})^{k_{f-2}}\varphi(\frac{q}{\gamma q})^{k_{f-1}}\varphi^2(\lambda_{f,\gamma})^{k_0}\varphi^3(\lambda_{f,\gamma})^{k_1}\cdots\varphi^{f+1}(\lambda_{f,\gamma})^{k_{f-1}},$$

$$g_{f-1}=(\frac{q}{\gamma q})^{k_{f-1}}\varphi(\lambda_{f,\gamma})^{k_0}\varphi^2(\lambda_{f,\gamma})^{k_1}\varphi^3(\lambda_{f,\gamma})^{k_2}\cdots\varphi^f(\lambda_{f,\gamma})^{k_{f-1}},$$

and Lemma 3.2 implies that $g_i\equiv 1 \bmod \pi$ for all i.

PROPOSITION 3.4. *We equip* $\mathbb{N}_{\vec{k},c}=\left(\mathcal{O}_E[[\pi]]^{|\tau|}\right)\eta$ *with semilinear* φ *and* Γ_K*-actions defined by* $\varphi(\eta)=(c\cdot q^{k_1},q^{k_2},...,q^{k_{f-1}},q^{k_0})\eta$ *and* $\gamma(\eta)=(g_1^{\gamma}(\pi),g_2^{\gamma}(\pi),...g_{f-1}^{\gamma}(\pi),g_0^{\gamma}(\pi))\eta$ *for the* $g_i(\pi)=g_i^{\gamma}(\pi)$ *defined above, where* $c\in\mathcal{O}_E^{\times}$*. The module* $\mathbb{N}_{\vec{k},c}$ *is a Wach module over* $\mathcal{O}_E[[\pi]]^{|\tau|}$ *with labeled Hodge-Tate weights* $\{-k_i\}_{\tau_i}$*. Moreover,* $\mathbb{D}_{\vec{k},c}\simeq E^{|\tau|}\bigotimes_{\mathcal{O}_E^{|\tau|}}\left(\mathbb{N}_{\vec{k},c}/\pi\mathbb{N}_{\vec{k},c}\right)$ *as filtered* φ*-modules over* $E^{|\tau|}$*, where* $\mathbb{D}_{\vec{k},c}=\left(E^{|\tau|}\right)\eta$ *is the filtered* φ*-module with Frobenius endomorphism* $\varphi(\eta)=(c\cdot p^{k_1},p^{k_2},...,p^{k_{f-1}},p^{k_0})\eta$ *and filtration*

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}_{\vec{k},c})=\begin{cases}E^{|\tau_{I_0}|}\eta & \text{if } j\le w_0,\\ E^{|\tau_{I_1}|}\eta & \text{if } 1+w_0\le j\le w_1,\\ \quad\cdots\cdots & \\ E^{|\tau_{I_{t-1}}|}\eta & \text{if } 1+w_{t-2}\le j\le w_{t-1},\\ \quad 0 & \text{if } j\ge 1+w_{t-1}.\end{cases}$$

Proof. (i) To prove that Γ_K acts on $\mathbb{N}_{\vec{k},c}$, it suffices to prove that $g_i^{\gamma_1\gamma_2}(\pi)=g_i^{\gamma_1}\gamma_1(g_i^{\gamma_2})$ for all $\gamma_1,\gamma_2\in\Gamma_K$ and $i\in I_0$. This follows immediately from the cocycle relations

$$\frac{q}{\gamma_1\gamma_2(q)}=\frac{q}{\gamma_1(q)}\gamma_1\left(\frac{q}{\gamma_2(q)}\right)\text{ and }\lambda_{f,\gamma_1\gamma_2}=\lambda_{f,\gamma_1}\gamma_1(\lambda_{f,\gamma_2}),$$

and the definition of the $g_i^{\gamma}(\pi)$. Since $g_i^{\gamma}(\pi)\equiv 1 \bmod \pi$ for all $i\in I_0$, the action of Γ_K on $\mathbb{N}_{\vec{k},c}/\pi\mathbb{N}_{\vec{k},c}$ is trivial. (ii) Let $k=\max\{k_0,k_1,...,k_{f-1}\}$ and let $\varphi^*(\mathbb{N}_{\vec{k},c})$ be the $\mathcal{O}_E[[\pi]]^{|\tau|}$-linear span of the set $\varphi(\mathbb{N}_{\vec{k},c})$. Let $c_1=c^{-1}$ and $c_i=1$ if

$i \neq 1$. Since $q^k\eta = \sum_{i=0}^{f-1} \left(q^{k-k_i}c_i e_i\right)\varphi(\eta) \in \varphi^*(\mathbb{N}_{\vec{k},c})$, it follows that q^k kills $\mathbb{N}_{\vec{k},c}/\varphi^*(\mathbb{N}_{\vec{k},c})$. (iii) To compute the filtration of $\mathbb{N}_{\vec{k},c}$, we use the fact that $q^j \mid \varphi(x)$ if and only if $\pi^j \mid x$ for any $x \in \mathcal{O}_E[[\pi]]$. Let $x = (x_0, x_1, ..., x_{f-1})\eta \in \mathbb{N}_{\vec{k},c}$. By Theorem 2.4, $x \in \mathrm{Fil^j}\mathbb{N}_{\vec{k},c}$ if and only if $\varphi(x) \in q^j\mathbb{N}_{\vec{k},c}$ or equivalently $q^j \mid \varphi(x_i)q^{k_i}$ for all $i \in I_0$. If $j \leq k_i$ there are no restrictions on the x_i, whereas if $j > k_i$ this is equivalent to $x_i \equiv 0 \mathrm{mod}\ \pi^{j-k_i}$. Therefore,

$$e_i\mathrm{Fil^j}\mathbb{N}_{\vec{k},c} = \begin{cases} e_i\mathbb{N}_{\vec{k},c} & \text{if } j \leq k_i, \\ e_i\pi^{j-k_i}\mathcal{O}_E[[\pi]]\eta & \text{if } j \geq 1+k_i. \end{cases}$$

This implies that

$$E^{|\tau|}\bigotimes_{\mathcal{O}_E^{|\tau|}} e_i\mathrm{Fil^j}\left(\mathbb{N}_{\vec{k},c}/\pi\mathbb{N}_{\vec{k},c}\right) = \begin{cases} e_iE^{|\tau|}\overline{\eta} & \text{if } j \leq k_i, \\ 0 & \text{if } j \geq 1+k_i. \end{cases}$$

For the filtration, we have

$$E^{|\tau|}\bigotimes_{\mathcal{O}_E^{|\tau|}} \mathrm{Fil^j}\left(\mathbb{N}_{\vec{k},c}/\pi\mathbb{N}_{\vec{k},c}\right) = \bigoplus_{i=0}^{f-1}\left(E^{|\tau|}\bigotimes_{\mathcal{O}_E^{|\tau|}} e_i\mathrm{Fil^j}(\mathbb{N}_{\vec{k},c}/\pi\mathbb{N}_{\vec{k},c})\right).$$

Recall from Notation 1.2 that after ordering the weights k_i and omitting possibly repeated weights we get $w_0 < w_1 < ... < w_{t-1}$. By the formulas above,

$$\mathrm{Fil^j}(\mathbb{D}_{\vec{k},c}) = \begin{cases} E^{|\tau|}\left(\sum_{i\in I_0} e_i\right)\eta & \text{if } \ j \leq w_0, \\ E^{|\tau|}\left(\sum_{\{i\in I_0:k_i>w_0\}} e_i\right)\eta & \text{if } \ 1+w_0 \leq j \leq w_1, \\ E^{|\tau|}\left(\sum_{\{i\in I_0:k_i>w_1\}} e_i\right)\eta & \text{if } \ 1+w_1 \leq j \leq w_2 \\ \cdots\cdots & \\ E^{|\tau|}\left(\sum_{\{i\in I_0:k_i>w_{t-2}\}} e_i\right)\eta & \text{if } 1+w_{t-2} \leq j \leq w_{t-1}, \\ 0 & \text{if } j \geq 1+w_{t-1}. \end{cases}$$

The formula for the filtration follows immediately, recalling that $I_j = \{i \in I_0 : k_i > w_{j-1}\}$ for each $j = 1, 2, ..., t-1$, and $E^{|\tau_{I_r}|} := E^f\left(\sum_{i\in I_r} e_i\right)$ for each $r = 0, 1, ..., t-1$. The isomorphism of filtered φ-modules is obvious. ☐

PROPOSITION 3.5. *Let $k_0, k_1, ..., k_{f-1}$ be arbitrary integers.*

(i) The weakly admissible rank one filtered φ-modules over $E^{|\tau|}$ with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$ are of the form $\mathbb{D}_{\vec{k},\vec{\alpha}} = \left(E^{|\tau|}\right)\eta$, with $\varphi(\eta) = (\alpha_0, \alpha_1, ..., \alpha_{f-1})\eta$ for some $\vec{\alpha} = (\alpha_0, \alpha_1, ..., \alpha_{f-1}) \in (E^{\times})^{|\tau|}$ such that $\mathrm{v_p}(\mathrm{Nm}_{\varphi}(\vec{\alpha})) = \sum\limits_{i\in I_0} k_i$ and

$$\mathrm{Fil^j}(\mathbb{D}_{\vec{k},\vec{\alpha}}) = \begin{cases} E^{|\tau_{I_0}|}\eta & \text{if } j \leq w_0, \\ E^{|\tau_{I_1}|}\eta & \text{if } 1+w_0 \leq j \leq w_1, \\ & \cdots\cdots \\ E^{|\tau_{I_{t-1}}|}\eta & \text{if } 1+w_{t-2} \leq j \leq w_{t-1}, \\ 0 & \text{if } j \geq 1+w_{t-1}. \end{cases}$$

(ii) The filtered φ-modules $\mathbb{D}_{\vec{k},\vec{\alpha}}$ and $\mathbb{D}_{\vec{v},\vec{\beta}}$ are isomorphic if and only if $\vec{k} = \vec{v}$ and $\mathrm{Nm}_{\varphi}(\vec{\alpha}) = \mathrm{Nm}_{\varphi}(\vec{\beta})$.

Proof. Follows easily arguing as in [Dou10], §§4 and 6. □

Corollary 3.6. *All the effective crystalline E-characters of G_K are those constructed in Proposition 3.4.*

Let $c \in \mathcal{O}_E^{\times}$ and $\vec{k} = (-k_1, -k_2, ..., -k_{f-1}, -k_0)$. We denote by $\chi_{c,\vec{k}}$ the crystalline character of G_K corresponding to the Wach module $\mathbb{N}_{\vec{k},c} = \left(\mathcal{O}_E[[\pi]]^{|\tau|}\right)\eta$ with φ action defined by $\varphi(e) = (c\cdot q^{k_1}, q^{k_2}, ..., q^{k_{f-1}}, q^{k_0})\eta$ and the unique commuting with it Γ_K-action defined in Proposition 3.4. When $c = 1$ we simply write $\chi_{\vec{k}}$. By Proposition 3.4 the crystalline character $\chi_i := \chi_{e_i}$ has labeled Hodge-Tate weights $-e_{i+1}$ for all i. By taking tensor products we see that $\chi_{c,\vec{k}} = \chi_{c,\vec{0}} \cdot \chi_0^{k_1} \cdot \chi_1^{k_2} \cdot \cdots \cdot \chi_{f-2}^{k_{f-1}} \cdot \chi_{f-1}^{k_0}$. As usual, we denote by Frob_p be the geometric Frobenius of $G_{\mathbb{Q}_p}$ and by Frob_K the geometric Frobenius of G_K. We have the following.

Lemma 3.7. *(i) The unramified character of G_{K_f} which maps Frob_{K_f} to c equals $\chi_{c,\vec{0}}$ for any $c \in \mathcal{O}_E^{\times}$;*

(ii) For any $i = 0, 1, ..., f-1$, $(\chi_i)_{|G_{K_{2f}}} = \chi_i \cdot \chi_{i+f}$, where the character on the left hand side is a character of G_{K_f} and the characters on the right hand side are characters of $G_{K_{2f}}$;

(iii) If χ is a crystalline character of G_{K_f} with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$, $i = 0, 1, ..., f-1$, its restriction to $G_{K_{2f}}$ has labeled weights $\{-k_i\}_{\tau_i}$, $i = 0, 1, ..., 2f-1$, with $k_{i+f} = k_i$ for all $i = 0, 1, ..., f-1$;

(iv) If χ and ψ are crystalline characters of G_{K_f}, then $\chi_{|G_{K_{df}}} = \psi_{|G_{K_{df}}}$ if and only if $\chi = \eta \cdot \psi$, where η is an unramified character of G_{K_f} which maps Frob_{K_f} to a d-th root of unity.

Proof. (i) Let $\sqrt[f]{c}$ be any choice of an f-th root of c in E. The filtered φ-module with trivial filtration and $\varphi(e) = \sqrt[f]{c} \cdot e$ corresponds to the unramified character η of $G_{\mathbb{Q}_p}$ which maps Frob_p to $\sqrt[f]{c}$. Since the $\mathrm{Frob}_{K_f} = (\mathrm{Frob}_p)^f_{|K_f}$, the restriction of η_c of η to K_f maps Frob_{K_f} to c. By Proposition 2.6 the rank one filtered φ-module corresponding to the unramified character η_c has trivial filtration and Frobenius $\varphi(e) = (\sqrt[f]{c}, \sqrt[f]{c}, ..., \sqrt[f]{c})\, e$, and by Proposition 3.5(ii) the latter is isomorphic to the rank one filtered φ-module with trivial filtration and $\varphi(e) = (c, 1, ...1)\, e$. Part (ii) follows from the definition of the characters χ_i and Proposition 2.6. Part (iii) follows immediately from part (ii). For part (iv) it suffices to prove that any crystalline character η of G_{K_f} with trivial restriction to $G_{K_{df}}$ is an unramified character of G_{K_f} which maps Frob_{K_f} to a d-th root of unity. The restriction of η to $G_{K_{df}}$ has all its labeled Hodge-Tate weights equal to zero, and by Corollary 2.7 so does η. By part (i) η is an unramified character of G_{K_f} which maps Frob_{K_f} to some constant, say c. The restriction of η to $G_{K_{df}}$ is trivial and maps $\mathrm{Frob}_{K_{df}} = \left(\mathrm{Frob}_{K_f}\right)^d_{|K_{df}}$ to c^d, therefore c is a d-th root of unity and part (iv) follows. □

Let χ be any E-character of G_K, and let $h \in G_{\mathbb{Q}_p}$. Since K is unramified over $\mathbb{Q}_p$, it is h-stable and the character χ^h with $\chi^h(g) := \chi\left(hgh^{-1}\right)$ is well defined. We have $h_{|K} =: \sigma_K^{n(h)}$ for a unique integer $n(h)$ modulo f. We denote by $\mathrm{T}(\chi)$ the rank one $\mathcal{O}_E$-representation of G_K defined by $\gamma e = \chi(\gamma)\, e$ for any basis element e and any $\gamma \in G_K$.

Lemma 3.8. *Let χ be the crystalline character corresponding to the Wach module defined in Proposition 3.4, and let $h \in G_{\mathbb{Q}_p}$. Let $\eta_1 = \left(\bar{h}^{-1}_{|K}\right) \cdot \eta$. The rank one module $\mathbb{N}^h := \left(\mathcal{O}_E[[\pi]]^{|\tau|}\right) \eta_1$ endowed with semilinear Frobenius and Γ_K-actions defined by*

$$\begin{aligned} \varphi(\eta_1) &= \left(c \cdot q^{k_{f+1-n(h)}},\ q^{k_{f+2-n(h)}}, ...,\ q^{k_{2f-n(h)}}\right) \eta_1 \text{ and} \\ \gamma(\eta_1) &= \left(g^{h\gamma h^{-1}}_{f+1+n(h^{-1})},\ g^{h\gamma h^{-1}}_{f+2-n(h)}, ...,\ g^{h\gamma h^{-1}}_{2f-1-n(h)},\ g^{h\gamma h^{-1}}_{2f-n(h)}\right) \eta_1, \end{aligned}$$

where the indices are viewed modulo f, is a Wach module whose corresponding crystalline character is χ^h.

Proof. It is trivial to check that $\mathbb{N}^h$ with the above defined actions is a Wach module. By Theorems 2.2 and 2.4, $\mathrm{T}(\chi) \simeq \left(\mathbb{A}_{K,E} \otimes_{\mathbb{A}^+_{K,E}} \mathbb{N}(\mathrm{T}(\chi))\right)^{\varphi=1}$, hence there exists some $\alpha \in \mathbb{A}_{K,E}$ such that $\varphi(\alpha \otimes \eta) = \alpha \otimes \eta$ and $\gamma(\alpha \otimes \eta) = \chi(\gamma)(\alpha \otimes \eta)$ for all $\gamma \in G_K$. This is equivalent to

$$\varphi(\alpha) \cdot \xi^{-1}\left(c \cdot q^{k_1}, q^{k_2}, ..., q^{k_0}\right) \otimes \eta = \alpha \otimes \eta \text{ and} \tag{3.2}$$

$$\gamma(\alpha) \cdot \xi^{-1}\left(g_1^{\gamma}, g_2^{\gamma}, ...g_{f-1}^{\gamma}, g_0^{\gamma}\right) \otimes \eta = \chi(\gamma)\, \alpha \otimes \eta \tag{3.3}$$

for all $\gamma \in G_K$, where ξ is the isomorphism defined in formula 2.1. A little computation shows that for any $(x_0, x_1, ..., x_{f-1}) \in \mathcal{O}_E[[\pi]]^{|\tau|}$,

$$h^{-1}\left(\xi^{-1}(x_0, x_1, ..., x_{f-1})\right) = \xi^{-1}\left(x_{f-n(h)}, x_{f+1-n(h)}, ..., x_{2f-1-n(h)}\right). \tag{3.4}$$

Let $\alpha_1 := h^{-1}\alpha \in \mathbb{A}_{K,E}$. We show that $\varphi(\alpha_1 \otimes \eta_1) = \alpha_1 \otimes \eta_1$ and $\gamma(\alpha_1 \otimes \eta_1) = \chi^h(\gamma)(\alpha_1 \otimes \eta_1)$ for all $\gamma \in G_K$. Indeed,

$$\begin{aligned}\varphi(\alpha_1 \otimes \eta_1) &= \varphi\left(h^{-1}\alpha\right) \otimes \varphi(\eta_1)\\ &= h^{-1}\varphi(\alpha) \cdot \xi^{-1}\left(c \cdot q^{k_{f+1-n(h)}},\ q^{k_{f+2-n(h)}}\ ,...,\ q^{k_{2f-n(h)}}\right) \otimes \eta_1\\ &\overset{3.4}{=} h^{-1}\varphi(\alpha) \cdot h^{-1}\xi^{-1}\left(c \cdot q^{k_1}, q^{k_2}, ..., q^{k_{f-1}}, q^{k_0}\right) \otimes h^{-1}\eta\\ &\overset{3.2}{=} h^{-1}(\alpha \otimes \eta) = \alpha_1 \otimes \eta_1.\end{aligned}$$

Also,

$$\begin{aligned}\gamma(\alpha_1 \otimes \eta_1) &= \gamma\left(h^{-1}\alpha\right) \cdot \xi^{-1}\left(g_{f+1-n(h)}^{h\gamma h^{-1}},\ g_{f+2-n(h)}^{h\gamma h^{-1}}, ...,\ g_{2f-1-n(h)}^{h\gamma h^{-1}},\ g_{2f-n(h)}^{h\gamma h^{-1}}\right) \otimes \eta_1\\ &\overset{3.4}{=} h^{-1}\left(h\gamma h^{-1}\alpha \cdot \xi^{-1}\left(g_1^{h\gamma h^{-1}},\ g_2^{h\gamma h^{-1}}, ...,\ g_{f-1}^{h\gamma h^{-1}},\ g_f^{h\gamma h^{-1}}\right) \otimes \eta\right)\\ &\overset{3.3}{=} h^{-1}\left(\chi\left(h\gamma h^{-1}\right)\alpha \otimes \eta\right) = \chi^h(\gamma)(\alpha_1 \otimes \eta_1)\end{aligned}$$

for all $\gamma \in G_K$. By Theorems 2.2 and 2.4, it follows that the crystalline character which corresponds to $\mathbb{N}^h$ is χ^h. □

COROLLARY 3.9. *If χ is a crystalline E-characters of G_K with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$, the character χ^h is crystalline with labeled Hodge-Tate weights $\{-\ell_i\}_{\tau_i}$, where $\ell_i = k_{f+i-n(h)}$ for all i, with the indices $f+i-n(h)$ viewed modulo f.*

COROLLARY 3.10. *The representation*

$$V_{K_f} \simeq \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_0^{k_1} \cdot \chi_1^{k_2} \cdot \cdots \cdot \chi_{2f-2}^{k_{2f-1}} \cdot \chi_{2f-1}^{k_0}\right)$$

is crystalline. Moreover, V_{K_f} is irreducible if and only if $k_i \neq k_{i+f}$ for some $i \in \{0, 1, ..., f-1\}$.

Proof. Since $V_{K_{2f}}$ is crystalline, V_{K_f} is crystalline. The corollary follows from Mackey's irreducibility criterion and Corollary 3.9. □

PROPOSITION 3.11. *Let V_K be an irreducible two-dimensional crystalline E-representation of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$, whose restriction to $G_{K_{2f}}$ is reducible. There exist some unramified character η of G_{K_f} and some nonnegative integers ℓ_i, $i = 0, 1, ..., 2f-1$ with $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$ for all $i = 0, 1, ..., f-1$ and $\ell_i \neq \ell_{i+f}$ for some $i \in \{0, 1, ..., f-1\}$, such that*

$$V_{K_f} \simeq \eta \otimes \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}\right).$$

Proof. Let χ be a constituent of $V_{K_{2f}}$. By Corollary 3.6, $\chi = \chi_c \cdot \chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}$ for some $c \in \mathcal{O}_E^{\times}$ and some integers ℓ_i. Let η be the unramified character of G_{K_f} which maps Frob_{K_f} to $\sqrt[2]{c}$. Arguing as in the proof of Lemma 3.7(i) we see that the restriction of η to $G_{K_{2f}}$ is χ_c, hence $\chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-2}^{\ell_0}$ is a constituent of $\left(\eta^{-1} \otimes V_{K_f}\right)_{|K_{2f}}$. Since $\eta^{-1} \otimes V_{K_f}$ is irreducible,

$$\eta^{-1} \otimes V_{K_f} \simeq \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}\right)$$

by Frobenius reciprocity. By Mackey's formula and Corollary 3.9,

$$V_{K_{2f}} \simeq \left(\chi_c \cdot \chi_0^{\ell_1} \cdot \chi_1^{\ell_2} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{2f-1}} \cdot \chi_{2f-1}^{\ell_0}\right) \bigoplus \bigoplus \left(\chi_c \cdot \chi_0^{\ell_{1+f}} \cdot \chi_1^{\ell_{2+f}} \cdot \cdots \cdot \chi_{2f-2}^{\ell_{3f-1}} \cdot \chi_{2f-1}^{\ell_{3f}}\right),$$

where the indices of the exponents of the second summand are viewed modulo $2f$. By Corollary 2.7, the restricted representation $V_{K_{2f}}$ has labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$, $i = 0, 1, 2, ..., 2f-1$, where $k_{i+f} = k_i$ for all $i = 0, 1, ..., f-1$. The labeled Hodge-Tate weights of the direct sum of characters in formula 3 with respect to the embedding τ_i of K_{2f} to E are $\{-\ell_i, -\ell_{i+f}\}$ for all $i = 0, 1, 2, ..., 2f-1$, with the indices $i+f$ viewed modulo $2f$. Therefore $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$ for all $i = 0, 1, ..., f-1$. The rest of the proposition follows from Corollary 3.10. ☐

Proposition 3.12. *Up to twist by some unramified character, there exist precisely* 2^{f^+-1} *distinct isomorphism classes of irreducible crystalline two-dimensional* E*-representations of* G_{K_f} *with labeled Hodge-Tate weights* $\{0, -k_i\}_{\tau_i}$*, whose restriction to* $G_{K_{2f}}$ *is reducible.*

Proof. In Proposition 3.11, notice that $\ell_{i+f} = k_i - \ell_l$ for all $i = 0, 1, ..., f-1$. The corollary follows since $\mathrm{Ind}_{K_{2f}}^{K_f}(\chi) \simeq \mathrm{Ind}_{K_{2f}}^{K_f}(\psi)$ if and only if $\{\chi, \chi^h\} = \{\psi, \psi^h\}$, where h is any element in $G_{\mathbb{Q}_p}$ lifting a generator of $\mathrm{Gal}\left(K_{2f}/K_f\right)$. ☐

4 Families of effective Wach modules of arbitrary weight and rank

We extend the method used by Berger-Li-Zhu in [BLZ04] for two-dimensional crystalline representations of $G_{\mathbb{Q}_p}$, in order to construct families of Wach modules of effective crystalline representations of G_K of arbitrary rank. Fixing a basis, we need to exhibit matrices Π and G_γ such that $\Pi\varphi(G_\gamma) = G_\gamma\gamma(\Pi)$ for all $\gamma \in \Gamma_K$, with some additional properties imposed by Theorem 2.4. In the two-dimensional case, for representations of $G_{\mathbb{Q}_p}$ and for a suitable basis, it is trivial to write down such a matrix Π assuming that the valuation of the trace of Frobenius of the corresponding filtered φ-module is suitably large, and the

main difficulty is in constructing a Γ_K-action which commutes with Π. When $K \neq \mathbb{Q}_p$, finding a matrix Π which gives rise to a prescribed weakly admissible filtration seems to be already hard, even in the two-dimensional case. Assuming that such a matrix Π is available, it is usually very hard to explicitly write down the matrices G_γ. There are exceptions to this, for example some split-reducible two-dimensional crystalline representations. In the general case, instead of explicitly writing down the matrices G_γ we prove that such matrices exist using a successive approximation argument.
Let $\mathcal{S} = \{X_i \ ; \ i = 0, 1, ..., m-1\}$ be a set of indeterminates, were $m \geq 1$ is any integer. We extend the actions of φ and Γ_K defined in equations 2.2 and 2.3 on the ring $\mathcal{O}_E[[\pi]]^{|\tau|} := \prod_{\tau: K \hookrightarrow E} \mathcal{O}_E[[\pi]]$ to an action on $\mathcal{O}_E[[\pi, \mathcal{S}]]^{|\tau|} := \prod_{\tau: K \hookrightarrow E} \mathcal{O}_E[[\pi, \mathcal{S}]]$, by letting φ and Γ_K act trivially on each indeterminate X_i. We let φ and Γ_K act on the matrices of $M_n^{\mathcal{S}} := M_n(\mathcal{O}_E[[\pi, \mathcal{S}]]^{|\tau|})$ entry-wise for any integer $n \geq 2$. For any integer $s \geq 0$, we write $\vec{\pi}^s = (\pi^s, \pi^s, ..., \pi^s)$, and for any $\alpha \in \mathcal{O}_E[[\pi, \mathcal{S}]]$ and any vector $\vec{r} = (r_0, r_1, ..., r_{f-1})$ with nonnegative integer coordinates we write $\alpha^{\vec{r}} = (\alpha^{r_0}, \alpha^{r_1}, ..., \alpha^{r_{f-1}})$. As usual, we assume that k_i are nonnegative integers and we write $k := w_{t-1} = \max\{k_0, k_1, ..., k_{f-1}\}$. Let $\ell \geq k$ be any fixed integer. We start our constructions with the following lemma.

Lemma 4.1. *Let $\Pi_i = \Pi_i(\mathcal{S}),\ i = 0, 1, ..., f-1$ be matrices in $M_n(\mathcal{O}_E[[\pi, \mathcal{S}]])$ such that $\det(\Pi_i) = c_i q^{k_i}$, with $c_i \in \mathcal{O}_E[[\pi]]^\times$. We denote by $\Pi(\mathcal{S})$ the matrix $(\Pi_1, \Pi_2, ..., \Pi_{f-1}, \Pi_0)$ and view it as an element of $M_n^{\mathcal{S}}$ via the natural isomorphism $M_n^{\mathcal{S}} \simeq M_n(\mathcal{O}_E[[\pi, \mathcal{S}]])^{|\tau|}$. We denote by $P_i = P_i(\mathcal{S})$ the reduction of $\Pi_i \bmod \pi$ for all i. Assume that for each $\gamma \in \Gamma_K$ there exists a matrix $G_\gamma^{(\ell)} = G_\gamma^{(\ell)}(\mathcal{S}) \in M_n^{\mathcal{S}}$ such that:*

1. $G_\gamma^{(\ell)}(\mathcal{S}) \equiv \overrightarrow{Id} \bmod \vec{\pi}^\ell$;
2. $G_\gamma^{(\ell)}(\mathcal{S}) - \Pi(\mathcal{S})\varphi(G_\gamma^{(\ell)}(\mathcal{S}))\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^\ell M_n^{\mathcal{S}}$;
3. *There is no nonzero matrix $H \in M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$ such that $HU = p^{ft}UH$ for some $t > 0$, where $U = \mathrm{Nm}_\varphi(P)$ and $P = P(\mathcal{S}) = (P_1, P_2, ..., P_{f-1}, P_0)$;*
4. *For each $s \geq \ell + 1$ the operator*
$$H \longmapsto H - Q_f H(p^{f(s-1)} Q_f^{-1}) : M_n(\mathcal{O}_E[[\mathcal{S}]]) \longrightarrow M_n(\mathcal{O}_E[[\mathcal{S}]]), \quad (4.1)$$
where $Q_f = P_1 P_2 \cdots P_{f-1} P_0$, is surjective.

Then for each $\gamma \in \Gamma_K$ there exists a unique matrix $G_\gamma(\mathcal{S}) \in M_n^{\mathcal{S}}$ such that

(i) $G_\gamma(\mathcal{S}) \equiv \overrightarrow{Id} \bmod \vec{\pi}$ *and*

(ii) $\Pi(\mathcal{S})\varphi(G_\gamma(\mathcal{S})) = G_\gamma(\mathcal{S})\gamma(\Pi(\mathcal{S}))$.

Proof. Uniqueness*:* Suppose that both the matrices $G_\gamma(\mathcal{S})$ and $G'_\gamma(\mathcal{S})$ satisfy the conclusions of the lemma and let $H = G'_\gamma(\mathcal{S})G_\gamma(\mathcal{S})^{-1}$. We easily see that $H \in \vec{Id} + \vec{\pi}M_n^{\mathcal{S}}$ and $H\Pi(\mathcal{S}) = \Pi(\mathcal{S})\varphi(H)$. We'll show that $H = \vec{Id}$. We write $H = \vec{Id} + \pi^t H_t + \cdots$, where $H_t \in M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$ for some $t \geq 1$ and $\Pi(\mathcal{S}) = P + \pi P^{(1)} + \pi^2 P^{(2)} + \cdots$, and we will show that $H_t = 0$. Since $H\Pi(\mathcal{S}) = \Pi(\mathcal{S})\varphi(H)$, we have $(H - \vec{Id})\Pi(\mathcal{S}) = \Pi(\mathcal{S})\varphi(H - \vec{Id})$. We divide both sides of this equation by π^t using that $\varphi(\pi) = q\pi$, and reduce mod π. Since $q \equiv p \bmod \pi$, this gives $H_t P = p^t P\varphi(H_t)$ which implies that $H_t U = p^{ft} U\varphi^f(H_t)$, where $U = \mathrm{Nm}_\varphi(P)$. Since φ acts trivially on X_i and $\mathcal{O}_E$, the map φ^f acts trivially on $M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$. Therefore $H_t U = p^{ft} U H_t$ and $H_t = 0$ by assumption (iii) of the lemma.

Existence: Fix a $\gamma \in \Gamma_K$. By assumptions (i) and (ii) of the lemma, there exists a matrix $G_\gamma^{(\ell)} \in \vec{Id} + \vec{\pi}^\ell\ M_n^{\mathcal{S}}$ such that

$$G_\gamma^{(\ell)} - \Pi(\mathcal{S})\varphi(G_\gamma^{(\ell)})\gamma(\Pi(\mathcal{S})^{-1}) = \vec{\pi}^\ell R^{(\ell)}$$

for some matrix $R^{(\ell)} = R^{(\ell)}(\gamma) \in M_n^{\mathcal{S}}$. We shall prove that for each $s \geq \ell + 1$ there exist matrices $R^{(s)} = R^{(s)}(\gamma) \in M_n^{\mathcal{S}}$ and $G_\gamma^{(s)} \in M_n^{\mathcal{S}}$ such that $G_\gamma^{(s)} \equiv G_\gamma^{(s-1)} \bmod \vec{\pi}^{s-1}M_n^{\mathcal{S}}$ and $G_\gamma^{(s)} - \Pi(\mathcal{S})\varphi(G_\gamma^{(s)})\gamma(\Pi(\mathcal{S})^{-1}) = \vec{\pi}^s R^{(s)}$. Let $G_\gamma^{(s)} = G_\gamma^{(s-1)} + \vec{\pi}^{s-1}H^{(s)}$, where $H^{(s)} \in M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$ and write $R^{(s)} = \bar{R}^{(s)} + \vec{\pi}\cdot C$ with $C \in M_n^{\mathcal{S}}$. We need

$$\left(G_\gamma^{(s-1)} + \vec{\pi}^{(s-1)}H^{(s)}\right) - \Pi(\mathcal{S})\left(\varphi(G_\gamma^{(s-1)}) + \varphi\,(\vec{\pi})^{(s-1)}\varphi\left(H^{(s)}\right)\right)\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^s M_n^{\mathcal{S}},$$

or equivalently

$$\begin{aligned} &G_\gamma^{(s-1)} - \Pi(\mathcal{S})\varphi(G_\gamma^{(s-1)})\gamma(\Pi(\mathcal{S})^{-1}) + \vec{\pi}^{(s-1)}H^{(s)} - \\ &- (\vec{q\pi})^{(s-1)}\Pi(\mathcal{S})\varphi\left(H^{(s)}\right)\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^s M_n^{\mathcal{S}}. \end{aligned}$$

The latter is equivalent to

$$\vec{\pi}^{(s-1)}R^{(s-1)} + \vec{\pi}^{(s-1)}H^{(s)} - (\vec{q\pi})^{(s-1)}\Pi(\mathcal{S})\varphi\left(H^{(s)}\right)\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^s M_n^{\mathcal{S}},$$

which is in turn equivalent to

$$H^{(s)} - \vec{q}^{(s-1)}\Pi(\mathcal{S})\varphi\left(H^{(s)}\right)\gamma(\Pi(\mathcal{S})^{-1}) \equiv -R^{(s-1)} \bmod \vec{\pi}M_n^{\mathcal{S}}.$$

This holds if and only if

$$H^{(s)} - \vec{p}^{(s-1)}P(\mathcal{S})\,\varphi\left(H^{(s)}\right)P(\mathcal{S})^{-1} = -\bar{R}^{(s-1)}. \tag{4.2}$$

Notice that $\vec{p}^{(s-1)}P(\mathcal{S})^{-1} \in M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$ since $s-1 \geq \ell \geq k = \max\{k_0, k_1, ..., k_{f-1}\}$. We write

$$H^{(s)} = \left(H_1^{(s)}, H_2^{(s)}, ..., H_{f-1}^{(s)}, H_0^{(s)}\right)$$

and

$$-\bar{R}^{(s-1)}=\left(\bar{R}_1^{(s-1)},\bar{R}_2^{(s-1)},...,\bar{R}_{f-1}^{(s-1)},\bar{R}_0^{(s-1)}\right).$$

Equation 4.2 is equivalent to the system of equations in $M_n\left(\mathcal{O}_E\left[[\mathcal{S}]\right]\right)$

$$H_i^{(s)}-P_i\cdot H_{i+1}^{(s)}\cdot\left(p^{s-1}P_i^{-1}\right)=\bar{R}_i^{(s-1)}, \tag{4.3}$$

where $i=1,2,...,f$, with indices viewed mod f. These imply that

$$H_1^{(s)}-Q_fH_1^{(s)}(p^{f(s-1)}Q_f^{-1})=\bar{R}_1^{(s-1)}+Q_1\bar{R}_2^{(s-1)}(p^{(s-1)}Q_1^{-1})+$$
$$+Q_2\bar{R}_3^{(s-1)}(p^{2(s-1)}Q_2^{-1})+\cdots+Q_{f-1}\bar{R}_0^{(s-1)}(p^{(s-1)(f-1)}Q_{f-1}^{-1}),$$

where $Q_i=P_1\cdots P_i$ for all $i=1,2,...,f$. From equations 4.3 we see that the matrices $H_i^{(s)}$, $i=2,3,...,f,$ are uniquely determined by the matrix $H_1^{(s)}$, so it suffices to prove that the operator defined in formula 4.1 contains

$$A=\bar{R}_1^{(s-1)}+Q_1\bar{R}_2^{(s-1)}(p^{(s-1)}Q_1^{-1})+Q_2\bar{R}_3^{(s-1)}(p^{2(s-1)}Q_2^{-1})+\cdots$$
$$+Q_{f-1}\bar{R}_0^{(s-1)}(p^{(s-1)(f-1)}Q_{f-1}^{-1})$$

in its image. Since $p^{i(s-1)}Q_i^{-1}\in M_n\left(\mathcal{O}_E\left[[\mathcal{S}]\right]\right)$ for all i, this is true by assumption (iv) of the lemma. We define $G_\gamma(\mathcal{S})=\lim\limits_{s\to\infty}G_\gamma^{(s)}(\mathcal{S})$ and the proof is complete. □

Let $\widetilde{M_n}$ be the ring $M_n\left(\mathcal{O}_E\left[[\mathcal{S}]\right]\right)/I$ where I is the ideal of $M_n\left(\mathcal{O}_E\left[[\mathcal{S}]\right]\right)$ generated by the set $\{p\cdot Id,\ X_i\cdot Id:\ X_i\in\mathcal{S}\}$. We use the notation of Lemma 4.1 and its proof, and we are interested in the image of the operator $\overline{H}\mapsto\overline{H-Q_fH(p^{f\ell}Q_f^{-1})}:\widetilde{M_n}\to\widetilde{M_n}$ where bar denotes reduction modulo I.

Proposition 4.2. *If the operator*

$$\overline{H}\mapsto\overline{H-Q_fH(p^{f\ell}Q_f^{-1})}:\widetilde{M_n}\to\widetilde{M_n} \tag{4.4}$$

is surjective, then for each $s\geq\ell+1$ the operator defined in formula 4.1 is surjective.

Proof. Case (i). $s\geq k+2$. In this case $f(s-1)-\sum\limits_{i=0}^{f-1}k_i\geq f\left(s-1-k\right)\geq f\geq1$. Since $Q_f^{-1}=P_0^{-1}P_{f-1}^{-1}P_{f-2}^{-1}...P_1^{-1}$ and $\det(P_i)=\bar{c}_ip^{k_i}$, it follows that $p^{f(s-1)}Q_f^{-1}\in pM_n(\mathcal{O}_E[[\mathcal{S}]])$. Let B be any matrix in $M_n\left(\mathcal{O}_E\left[[\mathcal{S}]\right]\right)$. We write

$$B=B-Q_fB\left(p^{f(s-1)}Q_f^{-1}\right)+pB_1$$

for some matrix $B_1\in M_n\left(\mathcal{O}_E\left[[\mathcal{S}]\right]\right)$. Similarly,

$$B_1=B_1-Q_fB_1\left(p^{f(s-1)}Q_f^{-1}\right)+pB_2$$

for some matrix $B_2 \in M_n(\mathcal{O}_E[[\mathcal{S}]])$ and

$$B = (B + pB_1) - Q_f(B + pB_1)\left(p^{f(s-1)}Q_f^{-1}\right) + p^2 B_2.$$

Continuing in the same fashion we get

$$B = \left(\sum_{i=0}^{N} p^i B_i\right) - Q_f\left(\sum_{i=0}^{N} p^i B_i\right)\left(p^{f(s-1)}Q_f^{-1}\right) + p^{N+1}B_{N+1}$$

for some matrix $B_{N+1} \in M_n(\mathcal{O}_E[[\mathcal{S}]])$ with $B_0 = B$. Let $H = \sum_{i=0}^{\infty} p^i B_i$. Then $H \in M_n(\mathcal{O}_E[[\mathcal{S}]])$ and $B = H - Q_f H\left(p^{f(s-1)}Q_f^{-1}\right)$.

Case (ii). $\ell = k$ and $s = k+1$. We reduce modulo the ideal I defined before Proposition 4.2. Let A be any element of $M_n(\mathcal{O}_E[[\mathcal{S}]])$. The operator

$$\overline{H} \longmapsto \overline{H - Q_f H\left(p^{f\ell}Q_f^{-1}\right)} : \widetilde{M_n} \to \widetilde{M_n}$$

contains $\bar{A} = A \bmod I$ in its image by the assumption of the lemma. Let $A = A_0 - Q_f A_0\left(p^{f\ell}Q_f^{-1}\right) \bmod I$ for some matrix $A_0 \in M_n(\mathcal{O}_E[[\mathcal{S}]])$. We write

$$A = A_0 - Q_f A_0\left(p^{f\ell}Q_f^{-1}\right) + pB_m + X_0 B_0 + \cdots + X_{m-1}B_{m-1}$$

for matrices $B_i \in M_n(\mathcal{O}_E[[\mathcal{S}]])$. Similarly $B_i = B_i^0 - Q_f B_i^0\left(p^{f\ell}Q_f^{-1}\right) \bmod I$ for matrices $B_i^0 \in M_n(\mathcal{O}_E[[\mathcal{S}]])$ and for all i. Then

$$\begin{aligned} A = A_0 - Q_f A_0\left(p^{f\ell}Q_f^{-1}\right) + pB_m^0 - Q_f\left(pB_m^0\right)\left(p^{f\ell}Q_f^{-1}\right) + \\ + X_0 B_1^0 - Q_f\left(X_0 B_1^0\right)\left(p^{f\ell}Q_f^{-1}\right) + \\ + \cdots + X_{m-1}B_{m-1}^0 - Q_f\left(X_{m-1}B_{f-1}^0\right)\left(p^{f\ell}Q_f^{-1}\right) \bmod I^2, \end{aligned}$$

therefore

$$\begin{aligned} A = {} & (A_0 + pB_m^0 + X_0 B_1^0 + \cdots + X_{m-1}B_{m-1}^0) - \\ & - Q_f(A_0 + pB_m^0 + X_0 B_1^0 + \cdots + X_{f-1}B_{m-1}^0)\left(p^{f\ell}Q_f^{-1}\right) \bmod I^2. \end{aligned}$$

By induction, $A = H - Q_f H\left(p^{f\ell}Q_f^{-1}\right)$ for some $H \in M_n(\mathcal{O}_E[[\mathcal{S}]])$. □

The surjectivity assumption of Proposition 4.2 is usually trivial to check thanks to the following proposition.

Proposition 4.3. *Assume that $\ell > k$ or $\ell = k$ and the weights k_i are not all equal. Then the operator defined in formula 4.4 is surjective.*

Proof. The proposition follows immediately because $\det Q_f = \bar{c}p^{k_1+k_2+\cdots+k_f}$, where $\bar{c} = \bar{c}_1\bar{c}_2\cdots\bar{c}_f$, since $f\ell > k_1 + \cdots + k_f$ and $p \in I$. $\square$

The following lemma summarizes the results of this section. We use the notation of Lemma 4.1.

LEMMA 4.4. *Let $\ell \geq k$ be a fixed integer. We assume that for each $\gamma \in \Gamma_K$ there exists a matrix $G_\gamma^{(\ell)} = G_\gamma^{(\ell)}(\mathcal{S}) \in M_n^{\mathcal{S}}$ such that:*

1. $G_\gamma^{(\ell)}(\mathcal{S}) \equiv \overrightarrow{Id} \mathrm{mod}\ \vec{\pi}^{\ell}$;
2. $G_\gamma^{(\ell)}(\mathcal{S}) - \Pi(\mathcal{S})\varphi(G_\gamma^{(\ell)}(\mathcal{S}))\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^{\ell} M_n^{\mathcal{S}}$;
3. *There is no nonzero matrix $H \in M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$ such that $HU = p^{ft}UH$ for some $t > 0$;*
4. *If $\ell = k$ and $k = k_i$ for all i, we additionally assume that the operator*
$$\overline{H} \mapsto \overline{H - Q_f H(p^{f\ell}Q_f^{-1})} : \widetilde{M_n} \to \widetilde{M_n}$$
is surjective.

Then for each $\gamma \in \Gamma_K$ there exists a unique matrix $G_\gamma(\mathcal{S}) \in M_n^{\mathcal{S}}$ such that

(i) $G_\gamma(\mathcal{S}) \equiv \overrightarrow{Id} \mathrm{mod}\ \vec{\pi}$, *and*

(ii) $\Pi(\mathcal{S})\varphi(G_\gamma(\mathcal{S})) = G_\gamma(\mathcal{S})\gamma(\Pi(\mathcal{S}))$.

For any vector $\vec{a} = (a_0, a_1, ..., a_{f-1}) \in \mathfrak{m}_E^{|\mathcal{S}|}$ we denote by $\Pi(\vec{a}) = (\Pi_1(a_1), \Pi_2(a_2), ..., \Pi_{f-1}(a_{f-1}), \Pi_0(a_0))$ the matrix obtained from $\Pi(\mathcal{S}) = (\Pi_1(X_1), \Pi_2(X_2), ..., \Pi_{f-1}(X_{f-1}), \Pi_0(X_0))$ by substituting $a_i \in \mathfrak{m}_E$ in each indeterminate X_i of $\Pi_i(X_i)$.

PROPOSITION 4.5. *For any $\vec{a} = (a_0, a_1, ..., a_{f-1}) \in \mathfrak{m}_E^{|\mathcal{S}|}$ and any $\gamma_1, \gamma_2, \gamma \in \Gamma_K$, the following equations hold:*

(i) $G_{\gamma_1\gamma_2}(\vec{a}) = G_{\gamma_1}(\vec{a})\gamma_1(G_{\gamma_2}(\vec{a}))$ *and*

(ii) $\Pi(\vec{a})\varphi(G_\gamma(\vec{a})) = G_\gamma(\vec{a})\gamma(\Pi(\vec{a}))$.

Proof. Both matrices $G_{\gamma_1\gamma_2}(\mathcal{S})$ and $G_{\gamma_1}(\mathcal{S})\gamma_1(G_{\gamma_2}(\mathcal{S}))$ are $\equiv \overrightarrow{Id} \mathrm{mod}\ \vec{\pi}$ and are solutions in A of the equation $\Pi(\mathcal{S})\varphi(A) = A\gamma(\Pi(\mathcal{S}))$. They are equal by the uniqueness part of Lemma 4.1. The second equation follows from part (ii) of the same lemma. $\square$

For any vector $\vec{a} \in \mathfrak{m}_E^{|\mathcal{S}|}$ we equip the module $\mathbb{N}(\vec{a}) = \bigoplus_{i=1}^{n} \left(\mathcal{O}_E[[\pi]]^{|\tau|}\right)\eta_i$ with semilinear φ and Γ_K-actions defined by $(\varphi(\eta_1), \varphi(\eta_2), ..., \varphi(\eta_n)) = (\eta_1, \eta_2, ..., \eta_n)\Pi(\vec{a})$ and $(\gamma(\eta_1), \gamma(\eta_2), ..., \gamma(\eta_n)) = (\eta_1, \eta_2, ..., \eta_n)G_\gamma(\vec{a})$ for any $\gamma \in \Gamma_K$. Proposition 4.5 implies that $(\gamma_1\gamma_2)x = \gamma_1(\gamma_2 x)$ and $\varphi(\gamma x) = \gamma(\varphi(x))$ for all $x \in \mathbb{N}(\vec{a})$ and $\gamma, \gamma_1, \gamma_2 \in \Gamma_K$. Since $G_\gamma(\vec{a}) \equiv \overrightarrow{Id} \mathrm{mod}\ \vec{\pi}$, it follows that Γ_K acts trivially on $\mathbb{N}(\vec{a})/\pi\mathbb{N}(\vec{a})$.

Proposition 4.6. *For any* $\vec{a} \in \mathfrak{m}_E^{|\mathcal{S}|}$, *the module* $\mathbb{N}(\vec{a})$ *equipped with the* φ *and* Γ_K*-actions defined above is a Wach module over* $\mathcal{O}_E[[\pi]]^{|\tau|}$ *corresponding (by Theorem 2.4) to some* G_K*-stable* $\mathcal{O}_E$*-lattice inside some* n*-dimensional crystalline* E*-representation of* G_K *with Hodge-Tate weights in* $[-k;\ 0]$.

Proof. The only thing left to prove is that $q^k\mathbb{N}(\vec{a}) \subset \varphi^*(\mathbb{N}(\vec{a}))$. Since $\det(\Pi_i) = c_i q^{k_i}$ we have $\det \Pi(\vec{a}) = (c_1 q^{k_1}, c_2 q^{k_2}, ..., c_0 q^{k_0})$ and

$$\begin{aligned} & (q^k\eta_1, q^k\eta_2, ..., q^k\eta_n) \\ = \ & (\eta_1, \eta_2, ..., \eta_n) \det \Pi(\vec{a}) \left(c_1^{-1}q^{k-k_1}, c_2^{-1}q^{k-k_2}, ..., c_0^{-1}q^{k-k_0}\right) \\ = \ & (\eta_1, \eta_2, ..., \eta_n) \left(\Pi(\vec{a}) \cdot \operatorname{adj}\left(\Pi(\vec{a})\right)\right) \left(c_1^{-1}q^{k-k_1}, c_2^{-1}q^{k-k_2}, ..., c_0^{-1}q^{k-k_0}\right) \\ = \ & (\varphi(\eta_1), \varphi(\eta_2), ..., \varphi(\eta_n)) \cdot (\operatorname{adj}\Pi(\vec{a})) \left(c_1^{-1}q^{k-k_1}, c_2^{-1}q^{k-k_2}, ..., c_0^{-1}q^{k-k_0}\right). \end{aligned}$$

Hence $(q^k\eta_1, q^k\eta_2, ..., q^k\eta_n) \in \varphi^*(\mathbb{N}(\vec{a}))$ and $q^k\mathbb{N}(\vec{a}) \subset \varphi^*(\mathbb{N}(\vec{a}))$. ∎

We proceed to prove the main theorem concerning the modulo p reductions of the crystalline representations corresponding to the families of Wach modules constructed in Proposition 4.6. By reduction modulo p we mean reduction modulo the maximal ideal $\mathfrak{m}_E$ of the ring of integers of the coefficient field E. If T is a G_K-stable $\mathcal{O}_E$-lattice in some E-linear representation V of G_K, we denote by $\overline{V} = k_E \bigotimes_{\mathcal{O}_E} \mathrm{T}$ the reduction of V modulo p, where k_E is the residue field of $\mathcal{O}_E$. The reduction $\overline{V}$ depends on the choice of the lattice T, and a theorem of Brauer and Nesbitt asserts that the semisimplification

$$\overline{V}^{s.s.} = \left(k_E \bigotimes_{\mathcal{O}_E} \mathrm{T}\right)^{s.s.}$$

is independent of T. Instead of the precise statement "there exist G_K-stable $\mathcal{O}_E$-lattices T_V and T_W inside the E-linear representation V and W of G_K respectively, such that $k_E \bigotimes_{\mathcal{O}_E} \mathrm{T}_V \simeq k_E \bigotimes_{\mathcal{O}_E} \mathrm{T}_W$", we abuse notation and write $\overline{V} \simeq \overline{W}$. For each $\vec{a} \in \mathfrak{m}_E^{|\mathcal{S}|}$, let $V(\vec{a}) = E \otimes_{\mathcal{O}_E} \mathrm{T}(\vec{a})$, where $\mathrm{T}(\vec{a}) = \mathbb{T}(\mathbb{D}(\vec{a}))$, and $\mathbb{D}(\vec{a}) = \mathbb{A}_{K,E} \bigotimes_{\mathbb{A}_{K,E}^+} \mathbb{N}(\vec{a})$. The representations $V(\vec{a})$ are n-dimensional crystalline E-representations of G_K with Hodge-Tate weights in $[-k;\ 0]$. Concerning their mod p reductions, we have the following theorem.

Theorem 4.7. *For any* $\vec{a} \in \mathfrak{m}_E^{|\mathcal{S}|}$, *the isomorphism* $\overline{V}(\vec{a}) \simeq \overline{V}(\vec{0})$ *holds.*

Proof. We prove that the k_E-linear representations $k_E \bigotimes_{\mathcal{O}_E} \mathrm{T}(\vec{a})$ and $k_E \bigotimes_{\mathcal{O}_E} \mathrm{T}(\vec{0})$ of G_K are isomorphic. Since $\Pi(\mathcal{S})$ and $G_\gamma(\mathcal{S}) \in M_n^{\mathcal{S}}$, we have $G_\gamma(\vec{a}) \equiv G_\gamma(\vec{0}) \bmod \mathfrak{m}_E$ and $\Pi(\vec{a}) \equiv \Pi(\vec{0}) \bmod \mathfrak{m}_E$. As (φ, Γ_K)-modules over $k_E((\pi))^{|\tau|}$, $\mathbb{D}(\vec{a})/\mathfrak{m}_E\mathbb{D}(\vec{a}) \simeq \mathbb{D}(\vec{0})/\mathfrak{m}_E\mathbb{D}(\vec{0})$. Hence $\mathbb{T}\left(\mathbb{D}(\vec{a})/\mathfrak{m}_E\mathbb{D}(\vec{a})\right) \simeq \mathbb{T}\left(\mathbb{D}(\vec{0})/\mathfrak{m}_E\mathbb{D}(\vec{0})\right)$, where $\mathbb{T}$ is Fontaine's functor on representations mod $\mathfrak{m}_E$. Since Fontaine's functor is exact, $\mathbb{T}\left(\mathbb{D}(\vec{a})/\mathfrak{m}_E\mathbb{D}(\vec{a})\right) \simeq \mathrm{T}(\vec{a})/\mathfrak{m}_E\mathrm{T}(\vec{a})$ and $\mathrm{T}(\vec{a})/\mathfrak{m}_E\mathrm{T}(\vec{a}) \simeq \mathrm{T}(\vec{0})/\mathfrak{m}_E\mathrm{T}(\vec{0})$. ∎

5 Families of two-dimensional crystalline representations

The main difficulty in applying Lemma 4.4 is in constructing the matrices $G_{\gamma}^{(\ell)}(\mathcal{S})$ which satisfy conditions (1) and (2). Conditions (3) and (4) are usually easy to check. Throughout this section we retain the notations of Lemma 4.4. We denote by E_{ij} the 2×2 matrix with 1 in the (i,j)-entry and 0 everywhere else. Recall that $E_{ij}\cdot E_{kl}=\delta_{jk}\cdot E_{il}$, where δ is the Kronecker delta function. Also recall our assumption that at least one of the weights k_i is strictly positive.

Proposition 5.1. *The operator* $\overline{H}\mapsto\overline{H-Q_fH(p^{f\ell}Q_f^{-1})}:\widetilde{M}_2\to\widetilde{M}_2$ *is surjective, unless* $\ell=k,\ k=k_i$ *for all* i *and* $\bar{Q}_f\in\{E_{11},E_{22}\}$.

Proof. It is straightforward to check that $\bar{Q}_f=E_{ij}$ for some $i,j\in\{1,2\}$ and

$$p^{k\ell}Q_f^{-1}\text{mod } I=\begin{cases} E_{22} & \text{if } \bar{Q}_f=E_{11},\\ E_{11} & \text{if } \bar{Q}_f=E_{22},\\ -E_{12} & \text{if } \bar{Q}_f=E_{12},\\ -E_{21} & \text{if } \bar{Q}_f=E_{21}.\end{cases}$$

If $\bar{Q}_f=E_{11}$ (respectively E_{22}), the image is the set of matrices with zero $(1,2)$ (respectively $(2,1)$) entry, while if $\bar{Q}_f=E_{12}$ or $\bar{Q}_f=E_{21}$ the operator becomes

$$\begin{pmatrix} h_{11} & h_{12}\\ h_{21} & h_{22}\end{pmatrix}\longmapsto\begin{pmatrix} h_{11} & h_{12}+h_{21}\\ h_{21} & h_{22}\end{pmatrix}$$

and

$$\begin{pmatrix} h_{11} & h_{12}\\ h_{21} & h_{22}\end{pmatrix}\longmapsto\begin{pmatrix} h_{11} & h_{12}\\ h_{21}+h_{12} & h_{22}\end{pmatrix}$$

respectively and is clearly surjective. The proposition follows from Proposition 4.3. ∎

Lemma 5.2. *If the matrix* $Q_f=P_1P_2\cdots P_{f-1}P_f$ *(with* $P_f=P_0$*) does not have eigenvalues which are a scalar multiple of each other, then the matrix* $U=\mathrm{Nm}_{\varphi}(P)$, *where* $P=(P_1,P_2,...,P_{f-1},P_0)$, *satisfies condition* (3) *of Lemma 4.4.*

Proof. Let $H\in M_n(\mathcal{O}_E[[\mathcal{S}]]^{|\tau|})$ be a nonzero matrix such that $HU=p^{ft}UH$ for some $t>0$. We write $H=(H_1,H_2,...,H_f)$ and $U=(U_1,U_2,...,U_f)$. Since $P\cdot\varphi(U)\cdot P^{-1}=U$, we have $P_iU_{i+1}P_i^{-1}=U_i$ for all i. Since $Q_f=U_1$, none of the U_i has eigenvalues which are a scalar multiple of each other. If H is invertible then $U_1=Q_f$ has eigenvalues with quotient p^{ft} which contradicts the assumption of the lemma. If H is nonzero and not invertible, there exists an index i such that $H_iU_i=p^{ft}\,U_iH_i$ and $\mathrm{rank}\,(H_i)=1$. There also exists an invertible matrix B such that

$$BH_iB^{-1}=\begin{pmatrix}\alpha_{11} & 0\\ \alpha_{21} & 0\end{pmatrix}$$

with $(\alpha_{11}, \alpha_{21}) \neq (0,0)$. Let $\Gamma = BU_iB^{-1}$ and write $\Gamma = (\gamma_{ij})$. The equation $H_iU_i = p^{ft}U_iH_i$ is equivalent to $p^{ft}\Gamma BH_iB^{-1} = BH_iB^{-1}\Gamma$ which implies that $\gamma_{12} = 0$ and $p^{ft}\gamma_{11}\alpha_{11} = \alpha_{11}\gamma_{11}$. If $\alpha_{11} \neq 0$, then $\gamma_{11} = 0$ a contradiction since Γ is invertible. If $\alpha_{11} = 0$, then $p^{ft}\alpha_{21}\gamma_{22} = \alpha_{21}\gamma_{11}$ and $p^{ft}\gamma_{22} = \gamma_{11}$ (since $\alpha_{21} \neq 0$). Since $\gamma_{12} = 0$, the latter implies that Γ has two eigenvalues with quotient p^{ft}. This in turn implies that U_i and its conjugate $Q_f = U_1$ have eigenvalues with quotient p^{ft} and contradicts the assumption of the lemma. Hence $H = 0$. ☐

In the two-dimensional case, instead of checking condition (3) of Lemma 4.4 it is often more convenient to use following corollary.

Corollary 5.3. *If* $\mathrm{Tr}\,(Q_f) \notin \bar{\mathbb{Q}}_p$, *then the matrix* $U = \mathrm{Nm}_\varphi(P)$ *satisfies condition* (3) *of Lemma 4.4.*

Proof. Since the determinant of Q_f is a nonzero scalar, the eigenvalues of Q_f are a scalar multiple of each other if and only if $\mathrm{Tr}\,(Q_f)$ is a scalar. ☐

5.1 Families of rank two Wach modules

We now apply Lemma 4.4 for matrices Π_i as in the following definition.

Definition 5.4. *For a fixed integer* $\ell \geq k = \max\{k_0, k_1, ..., k_{f-1}\}$ *we define matrices of the following four types*

$$t_1\colon \begin{pmatrix} c_iq^{k_i} & 0 \\ X_i\varphi(z_i) & 1 \end{pmatrix},\ t_2\colon \begin{pmatrix} X_i\varphi(z_i) & 1 \\ c_iq^{k_i} & 0 \end{pmatrix},$$

$$t_3\colon \begin{pmatrix} 1 & X_i\varphi(z_i) \\ 0 & c_iq^{k_i} \end{pmatrix},\ t_4\colon \begin{pmatrix} 0 & c_iq^{k_i} \\ 1 & X_i\varphi(z_i) \end{pmatrix},$$

where X_i *is an indeterminate,* $c_i \in \mathcal{O}_E$, *and* z_i *is a polynomial of degree* $\leq \ell - 1$ *in* $\mathbb{Z}_p[\pi]$ *such that* $z_i \equiv p^{m_\ell} \mathrm{mod}\ \pi$, *where* $m_\ell := \lfloor \frac{\ell-1}{p-1} \rfloor$. *Matrices of type* t_1 *or* t_3 *are called of odd type while matrices of type* t_2 *or* t_4 *are called of even type. We write* $\Pi^{\vec{i}}(S) = (\Pi_1(X_1), \Pi_2(X_2), ..., \Pi_{f-1}(X_{f-1}), \Pi_0(X_0))$ *with* $\vec{i} = (i_1, i_2, ..., i_{f-1}, i_0)$ *the vector in* $\{1, 2, 3, 4\}^f$ *whose* j*-th coordinate* i_j *is the type of the matrix* Π_j *for all* $j \in I_0$. *We call* $\vec{i}$ *the type-vector attached to the matrix* f*-tuple* $\Pi^{\vec{i}}(S)$.

The polynomials z_i appearing in the entries of the matrices Π_i will be defined shortly. We will also define functions x_i^γ, $y_i^\gamma \in 1 + \pi\mathbb{Z}_p[[\pi]]$ such that

$$G_\gamma^{(\ell)} - \Pi(\mathcal{S})\varphi(G_\gamma^{(\ell)})\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^\ell M_2^{\mathcal{S}}$$

for all $\gamma \in \Gamma_K$, where

$$G_\gamma^{(\ell)} = \mathrm{diag}\left(\left(x_0^\gamma, x_1^\gamma, ..., x_{f-1}^\gamma\right), \left(y_0^\gamma, y_1^\gamma, ..., y_{f-1}^\gamma\right)\right).$$

Let

$$\Pi(\mathcal{S})=\begin{pmatrix}(\alpha_1,\alpha_2,...\alpha_{f-1},\alpha_0) & (\beta_1,\beta_2,...,\beta_{f-1},\beta_0)\\ (\gamma_1,\gamma_2,...,\gamma_{f-1},\gamma_0) & (\delta_1,\delta_2,...,\ \delta_{f-1},\delta_0)\end{pmatrix}\text{ with }\begin{pmatrix}\alpha_i & \beta_i\\ \gamma_i & \delta_i\end{pmatrix}$$

belonging to the set

$$\left\{\begin{pmatrix}c_iq^{k_i} & 0\\ X_i\varphi(z_i) & 1\end{pmatrix},\begin{pmatrix}X_i\varphi(z_i) & 1\\ c_iq^{k_i} & 0\end{pmatrix},\begin{pmatrix}1 & X_i\varphi(z_i)\\ 0 & c_iq^{k_i}\end{pmatrix},\begin{pmatrix}0 & c_iq^{k_i}\\ 1 & X_i\varphi(z_i)\end{pmatrix}\right\}.$$

For each $i=1,2,...,f$ we demand that all of the elements

$$x_{i-1}^{\gamma}-\frac{\alpha_i\varphi\left(x_i^{\gamma}\right)(\gamma\delta_i)-\beta_i\varphi\left(y_i^{\gamma}\right)(\gamma\gamma_i)}{\varepsilon_i\left(\gamma q\right)^{k_i}},\ \frac{\beta_i\varphi\left(y_i^{\gamma}\right)(\gamma\alpha_i)-\alpha_i\varphi\left(x_i^{\gamma}\right)(\gamma\beta_i)}{\varepsilon_i\left(\gamma q\right)^{k_i}},\tag{5.1}$$

$$y_{i-1}^{\gamma}-\frac{\delta_i\varphi\left(y_i^{\gamma}\right)(\gamma\alpha_i)-\gamma_i\varphi\left(x_i^{\gamma}\right)(\gamma\beta_i)}{\varepsilon_i\left(\gamma q\right)^{k_i}},\ \frac{\gamma_i\varphi\left(x_i^{\gamma}\right)(\gamma\delta_i)-\delta_i\varphi\left(y_i^{\gamma}\right)(\gamma\gamma_i)}{\varepsilon_i\left(\gamma q\right)^{k_i}}\tag{5.2}$$

of $\mathcal{O}_E[[\pi,X_0,...,X_{f-1}]][q^{-1}]$ which belong to $\mathcal{O}_E[[\pi]][q^{-1}]$ are zero, and those which contain an indeterminate belong to $\pi^{\ell}\mathcal{O}_E[[\pi,X_0,...,X_{f-1}]]$, where in the formulas above $\varepsilon_i=1$ if Π_i has type 1 or 3 and $\varepsilon_i=-1$ if Π_i has type 2 or 4. As usual lower indices are viewed modulo f.

Proposition 5.5. *For each i, equations 5.1 and 5.2 imply that*

$$x_{i-1}^{\gamma}=\left(\frac{q}{\gamma q}\right)^{\ell_i}\varphi\left(w_i^{\gamma}\right)\ \textit{and}\ y_{i-1}^{\gamma}=\left(\frac{q}{\gamma q}\right)^{\ell_i'}\varphi\left(\left(w_i^{\gamma}\right)'\right),\tag{5.3}$$

with $\ell_i\in\{0,k_i\},\ w_i^{\gamma}\in\{x_i^{\gamma},y_i^{\gamma}\},\ \ell_i'=k_i-\ell_i,$ *and* $\left(w_i^{\gamma}\right)'=\begin{cases}x_i^{\gamma}\text{ if }w_i^{\gamma}=y_i^{\gamma},\\ y_i^{\gamma}\text{ if }w_i^{\gamma}=x_i^{\gamma}.\end{cases}$

Proof. If Π_i is of type 1, then $\beta_i=0$, $\alpha_i=c_iq^{k_i}$ and $\delta_i=1$. We must have $q^{k_i}\varphi\left(x_i^{\gamma}\right)=x_{i-1}^{\gamma}\left(\gamma q\right)^{k_i}$ and $\varphi\left(y_i^{\gamma}\right)=y_{i-1}^{\gamma}$. The proposition holds with $\ell_i=k_i$, $w_i^{\gamma}=x_i^{\gamma}$, $\ell_i'=0$, and $\left(w_i^{\gamma}\right)'=y_i^{\gamma}$. The cases where Π_i is of type $2,3$, or 4 are identical. ☐

From Proposition 5.5 it follows that

$$x_0^{\gamma}=\left(\prod_{i=0}^{f-1}\varphi^i\left(\frac{q}{\gamma q}\right)^{s_i}\right)\varphi^f\left(z_f^{\gamma}\right)\text{ and }y_0^{\gamma}=\left(\prod_{i=0}^{f-1}\varphi^i\left(\frac{q}{\gamma q}\right)^{s_i'}\right)\varphi^f\left(\left(z_f^{\gamma}\right)'\right),\tag{5.4}$$

with $s_i',s_i\in\{\ell_i,\ell_i'\}$. If $z_f^{\gamma}=x_0^{\gamma}$, then $\left(z_f^{\gamma}\right)'=y_0^{\gamma}$, and by Lemma 3.3 equations 5.4 have unique $\equiv 1 \bmod \pi$ solutions given by

$$x_0^{\gamma}=\prod_{i=0}^{f-1}\varphi^i\left(\lambda_{f,\gamma}\right)^{s_i}\text{ and }y_0^{\gamma}=\prod_{i=0}^{f-1}\varphi^i\left(\lambda_{f,\gamma}\right)^{s_i'}.\tag{5.5}$$

If If $z_f^\gamma = y_0^\gamma$, then $\left(z_f^\gamma\right)' = x_0^\gamma$ and equations 5.4 imply that

$$x_0^\gamma = \prod_{i=0}^{f-1}\left(\varphi^i\left(\frac{q}{\gamma q}\right)^{s_i}\cdot\varphi^{i+f}\left(\frac{q}{\gamma q}\right)^{s_i'}\right)\varphi^{2f}\left(x_0^\gamma\right), \tag{5.6}$$

$$y_0^\gamma = \prod_{i=0}^{f-1}\left(\varphi^i\left(\frac{q}{\gamma q}\right)^{s_i'}\cdot\varphi^{i+f}\left(\frac{q}{\gamma q}\right)^{s_i}\right)\varphi^{2f}\left(y_0^\gamma\right), \tag{5.7}$$

which by Lemma 3.3 have unique $\equiv 1 \mathrm{mod}\ \pi$ solutions given by

$$x_0^\gamma = \prod_{i=0}^{f-1}\left(\varphi^i\left(\lambda_{2f,\gamma}\right)^{s_i}\cdot\varphi^{i+f}\left(\lambda_{2f,\gamma}\right)^{s_i'}\right), \tag{5.8}$$

$$y_0^\gamma = \prod_{i=0}^{f-1}\left(\varphi^i\left(\lambda_{2f,\gamma}\right)^{s_i'}\cdot\varphi^{i+f}\left(\lambda_{2f,\gamma}\right)^{s_i}\right). \tag{5.9}$$

Equations 5.3 for $i = f$ give the unique $\equiv 1 \mathrm{mod}\ \pi$ solutions for x_{f-1}^γ and y_{f-1}^γ, and continuing for $i = f-1, f-2, ..., 2$, we get the unique $\equiv 1 \mathrm{mod}\ \pi$ solutions for x_i^γ and y_i^γ. We now define the polynomials z_i so that for each $\gamma \in \Gamma_K$, the matrix $G_\gamma^{(\ell)} \equiv \overrightarrow{Id} \mathrm{mod}\ \vec{\pi}$ satisfies the congruence $G_\gamma^{(\ell)} - \Pi(\mathcal{S})\varphi(G_\gamma^{(\ell)})\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^\ell M_2^{\mathcal{S}}$.

Lemma 5.6. *Let $\mathcal{R} = \{\sum_{i\geq 0} a_i\pi^i \in \mathbb{Q}_p[[\pi]] : \mathrm{v_p}(a_i) + \frac{i}{p-1} \geq 0$ for all $i \geq 0\}$. The set $\mathcal{R}$ endowed with the addition and the multiplication of $\mathbb{Q}_p[[\pi]]$ is a subring of $\mathbb{Q}_p[[\pi]]$ which is stable under the φ and the Γ_K-actions. Moreover,*

(i) $(\frac{q_n}{p})^{\pm 1} \in \mathcal{R}$ for all $n \geq 1$ and $(\lambda_f)^{\pm 1} \in \mathcal{R}$ for all $f \geq 1$;

(ii) Let $b = cp^N b^*$, where $c \in \mathcal{O}_E^\times$, $n \in \mathbb{Z}$, and $b^* \in \mathcal{R}\setminus\{0\}$ is such that $\frac{b^*}{\gamma b^*} \in 1 + \pi\mathbb{Z}_p[[\pi]]$ for all $\gamma \in \Gamma_K$. If $\ell \geq 1$ is a fixed integer, there exists some polynomial $z = z(\ell, b) \in \mathbb{Z}_p[\pi]$ with $\deg_\pi z \leq \ell - 1$ and $z \equiv p^{m_\ell} \mathrm{mod}\ \pi$, where $m_\ell = \lfloor\frac{\ell-1}{p-1}\rfloor$, such that $z - \gamma z\frac{b}{\gamma b} \in \pi^\ell\mathbb{Z}_p[[\pi]]$ for all $\gamma \in \Gamma_K$.

Proof. We notice that the coefficients a_i of π^i in $\frac{q}{p}$ are such that $\mathrm{v_p}(a_i) + \frac{i}{p-1} \geq 0$ for all $i = 0, 1, ...$ Motivated by this we consider the set $\mathcal{R}$ of all functions of $\mathbb{Q}_p[[\pi]]$ with the same property. This is a ring with the obvious operations, stable under φ and Γ_K. One easily checks that $\left(\frac{p}{q}\right)^{\pm 1} \in \mathcal{R}$ and therefore $\left(\frac{q_n}{p}\right)^{\pm 1} \in \mathcal{R}$ for all $n \geq 1$ from which (i) follows easily. (ii) Since Γ_K acts trivially on $\mathcal{O}_E^\times$ we may replace b by $c^{-1}b$ and assume that $c = 1$. We write $b = p^n b^*$. Let $p^m b = z + a$, where $a \in \pi^\ell\mathbb{Q}_p[[\pi]]$ and $\deg_\pi z \leq \ell - 1$, for integer m which will be chosen large enough so that $z \in \mathbb{Z}_p[\pi]$. Let $z = \sum_{j=0}^{\ell-1} z_j\pi^j$. Since

$p^{m+n}b^{*}=z+a$ and $b^{*}\in\mathcal{R}$, we have $\mathrm{v_p}(z_j)-m-n+\frac{j}{p-1}\geq 0$ for all $j\geq 0$. We need $\mathrm{v_p}(z_j)>-1$ for all $j=0,1,...,\ell-1$ and it suffices to have $m+n-\frac{\ell-1}{p-1}>-1$. We choose $m=\lfloor\frac{\ell-1}{p-1}\rfloor-n$. Then $z\in\mathbb{Z}_p[\pi]$, $\deg_{\pi}z\leq\ell-1$ and $z\equiv p^{m+n}=p^{m_\ell}\mathrm{mod}\ \pi$, For any $\gamma\in\Gamma_K$, $z-\gamma z\frac{b}{\gamma b}=p^m b-a-b\gamma(b^{-1})\left(p^m(\gamma b)-\gamma a\right)=b\gamma(b^{-1})\gamma a-a\in\pi^{\ell}\mathbb{Q}_p[[\pi]]$. Since $z\in\mathbb{Z}_p[\pi]$ and $b\gamma(b^{-1})\in 1+\pi\mathbb{Z}_p[[\pi]]$, we have $z-\gamma z\frac{b}{\gamma b}\in\pi^{\ell}\mathbb{Z}_p[[\pi]]=\mathbb{Z}_p[[\pi]]\cap\pi^{\ell}\mathbb{Q}_p[[\pi]]$ for all $\gamma\in\Gamma_K$. □

LEMMA 5.7. *For any $\gamma\in\Gamma_K$ and $i\in I_0$,*

(i) $x_i^{\gamma},y_i^{\gamma}\in 1+\pi\mathbb{Z}_p[[\pi]]$;

(ii) $x_i^{\gamma}=\frac{a_i}{\gamma a_i}$ *and* $y_i^{\gamma}=\frac{b_i}{\gamma b_i}$ *for some a_i and b_i with* $(a_i)^{\pm1}$ *and* $(b_i)^{\pm1}\in\mathcal{R}$.

Proof. (i) is clear by the definition of the $x_i^{\gamma},y_i^{\gamma}$ and Lemma 3.2. (ii) Let $i=0$. If $z_f^{\gamma}=x_0^{\gamma}$, by equation 5.5 we have $x_0^{\gamma}=\frac{a_0}{\gamma a_0}$, where $a_0=\prod_{i=0}^{f-1}\varphi^i(\lambda_f)^{s_i}\in\mathcal{R}$. Since $(\lambda_f)^{\pm1}\in\mathcal{R}$ and $\mathcal{R}$ is φ-stable, $(a_0)^{\pm1}\in\mathcal{R}$. If $z_f^{\gamma}=y_0^{\gamma}$, by equation 5.8 we have $x_0^{\gamma}=\frac{a_0}{\gamma a_0}$, where $a_0=\prod_{i=0}^{f-1}\left(\varphi^i(\lambda_f)^{s_i}\varphi^{i+f}(\lambda_f)^{s_i'}\right)\in\mathcal{R}$, therefore $(a_0)^{\pm1}\in\mathcal{R}$. The proof for y_0^{γ} and $(b_i)^{\pm1}$ is similar. For x_{f-1}^{γ}, notice that $x_{f-1}^{\gamma}=\left(\frac{q}{\gamma q}\right)^{\ell_i}\varphi(w_i^{\gamma})=\frac{\gamma\left(\varphi(c_0)\left(\frac{q}{p}\right)^{\ell_f}\right)}{\varphi(c_0)\left(\frac{q}{p}\right)^{\ell_f}}$ with $c_0\in\{a_0,b_0\}$. Since $(a_0)^{\pm1},(b_0)^{\pm1}\in\mathcal{R}$, it follows that $x_{f-1}^{\gamma}\in\mathcal{R}$. Since $\left(\varphi(c_0)\left(\frac{q}{p}\right)^{\ell_f}\right)^{\pm1}\in\mathcal{R}$, it follows that $(a_{f-1})^{\pm1}\in\mathcal{R}$. Similarly y_{f-1}^{γ} and $(b_{f-1})^{\pm1}\in\mathcal{R}$. The lemma follows by induction. □

To define the polynomials z_i we will also need the following lemma.

LEMMA 5.8. *If $\alpha\in\pi^{\ell}\mathcal{O}_E[[\pi]]$ and $0\leq k\leq\ell$ is an integer, then* $\frac{\varphi(\alpha)}{(\gamma q)^k}\in\pi^{\ell}\mathcal{O}_E[[\pi]]$.

Proof. Since $\frac{\gamma q}{q}\equiv 1\mathrm{mod}\ \pi$, it suffices to prove that $\frac{\varphi(\alpha)}{q^k}\in\pi^{\ell}\mathcal{O}_E[[\pi]]$. Let $\alpha=\pi^{\ell}\beta$ for some $\beta\in\mathcal{O}_E[[\pi]]$. We have $\varphi\left(\frac{\alpha}{\pi^k}\right)=\varphi(\pi)^{\ell-k}\varphi(\beta)=q^{\ell-k}\pi^{\ell-k}\varphi(\beta)$. Hence $\frac{\varphi(\alpha)}{q^k}=\pi^k\varphi\left(\frac{\alpha}{\pi^k}\right)=\pi^k q^{\ell-k}\pi^{\ell-k}\varphi(\beta)=\pi^{\ell}q^{\ell-k}\varphi(\beta)\in\pi^{\ell}\mathcal{O}_E[[\pi]]$. □

PROPOSITION 5.9. *Let $k=\max\{k_0,k_1,...,k_{f-1}\}$, let $\ell\geq k$ be a fixed integer and let $m_\ell=\lfloor\frac{\ell-1}{p-1}\rfloor$. There exist polynomials $z_i\in\mathbb{Z}_p[\pi]$ with $\deg_{\pi}z_i\leq\ell-1$ such that $z_i\equiv p^{m_\ell}\mathrm{mod}\ \pi$ with the following properties:*

(i) $G_{\gamma}^{(\ell)}\equiv\overrightarrow{Id}\mathrm{mod}\ \vec{\pi}$;

(ii) $G_{\gamma}^{(\ell)}-\Pi(\mathcal{S})\varphi(G_{\gamma}^{(\ell)})\gamma(\Pi(\mathcal{S})^{-1})\in\vec{\pi}^{\ell}M_2^{\mathcal{S}}$ *for each $\gamma\in\Gamma_K$.*

Proof. Suppose that P_i is of type 2 and $\alpha_i = X_i\varphi(z_i)$ for some polynomial z_i to be defined. Then $\beta_i = 1$ and $\beta_i\varphi(y_i^\gamma) = x_{i-1}^\gamma(\gamma\beta_i)$ implies that $x_{i-1}^\gamma = \varphi(y_i^\gamma)$. We need

$$X_i\left(\varphi(z_i)\varphi(x_i^\gamma) - x_{i-1}^\gamma\varphi(\gamma z_i)\right)\frac{1}{(\gamma q)^{k_i}} \in \pi^\ell\mathcal{O}_E[[\pi, X_0, ..., X_{f-1}]]$$

for all $\gamma \in \Gamma_K$. By Lemma 5.8 it suffices to define z_i so that $z_i x_i^\gamma - y_i^\gamma\gamma z_i \in \pi^\ell\mathcal{O}_E[[\pi]]$ for all $\gamma \in \Gamma_K$. Since $x_i^\gamma \in 1 + \pi\mathbb{Z}_p[[\pi]]$ for all $\gamma \in \Gamma_K$, this is equivalent to $z_i - \frac{y_i^\gamma}{x_i^\gamma}\gamma z_i \in \pi^\ell\mathcal{O}_E[[\pi]]$. By Lemma 5.7 we have $\frac{y_i^\gamma}{x_i^\gamma} = \frac{b}{\gamma b}$, where $b = a_i(b_i)^{-1} \in \mathcal{R}$. Since $\frac{y_i^\gamma}{x_i^\gamma} \in 1 + \pi\mathbb{Z}_p[[\pi]]$, the existence of the z_i follows from Lemmata 5.6 and 5.7. The proof for P_i of type 1, 3 and 4 is identical. □

Proposition 5.10. *If $\alpha(\pi) = \sum_{n=0}^{\infty}\alpha_n\pi^n \in \mathbb{Q}_p[[\pi]]$ is such that $\mathrm{v_p}(\alpha_i) \geq 0$ for all $i = 0, 1, 2, ..., p-2$ and $\mathrm{v_p}(\alpha_{p-1}) > -1$, then the first $p-1$ coefficients of $\alpha(\pi)^p$ are in $\mathbb{Z}_p$. In particular, the first $p-1$ coefficients of the p-th power of any element of $\mathcal{R}$ are in $\mathbb{Z}_p$.*

Proof. Follows easily using the binomial expansion. □

Proposition 5.11. *If $k_i = p$ for all i, then there exist polynomials $z_i \in \mathbb{Z}_p[\pi]$ with $\deg_\pi z_i \leq p-1$ such that $z_i \equiv 1 \mathrm{mod}\ \pi$, and such that $G_\gamma^{(p)} - \Pi(\mathcal{S})\varphi(G_\gamma^{(p)})\gamma(\Pi(\mathcal{S})^{-1}) \in \vec{\pi}^p M_2^{\mathcal{S}}$ for any $\gamma \in \Gamma_K$.*

Proof. Assume that P_i is of type 2 and let x_0^γ and y_0^γ be as in the proof of Proposition 5.9. First we notice that the exponents s_i and s_i' in formulas 5.5 or 5.8 and 5.9 for the x_0^γ and y_0^γ are either 0 or p. With the notation of Lemma 5.7 we have $\frac{y_0^\gamma}{x_0^\gamma} = c_0\left(\gamma c_0^{-1}\right)$, where $c_0 = a_0^{-1}b_0$. The formulas for a_0^{-1} and b_0 in the proof of Lemma 5.7 imply that they are both p-th powers of elements of $\mathcal{R}$. From the same formulas and Lemma 3.2 it follows that $a_0^{-1}(0) = b_0(0) = 1$. By Lemma 5.10, $c_0 = z_0 + a$ for some polynomial $z_0 \in \mathbb{Z}_p[\pi]$ of degree $\leq p-1$ and constant term 1 and some $a \in \pi^p\mathbb{Q}_p[[\pi]]$. For any $\gamma \in \Gamma_K$, $z_0 - \frac{y_0^\gamma}{x_0^\gamma}\gamma z_0 = c_0 - a - c_0\left(\gamma c_0^{-1}\right)(\gamma c_0 - \gamma a) = c_0\left(\gamma c_0^{-1}\right)\gamma a - a \in \pi^p\mathbb{Q}_p[[\pi]]$. Since $\frac{y_0^\gamma}{x_0^\gamma} \in 1 + \pi\mathbb{Z}_p[[\pi]]$ and $z_0 \in \mathbb{Z}_p[\pi]$, $z_0 - \frac{y_0^\gamma}{x_0^\gamma}\gamma z_0 \in \mathbb{Z}_p[[\pi]] \cap \pi^p\mathbb{Q}_p[[\pi]] = \pi^p\mathbb{Z}_p[[\pi]]$. The proof for the other z_i is similar, using formulas 5.3 and noticing that $\left(\frac{q}{\gamma q}\right)^{\pm 1} \in 1 + \pi\mathbb{Z}_p[[\pi]]$. The proof for P_i of type 1, 3 or 4 is identical. □

Remark 5.12. *If $k_i = p$ for all i, then there exist polynomials $z_i \in \mathbb{Z}_p[\pi]$ with $\deg_\pi z_i \leq p-1$ and $z_i \equiv 1 \mathrm{mod}\ \pi$ which satisfy properties (i) and (ii) of Proposition 5.9. This follows immediately from Proposition 5.11.*

Next, we explicitly determine when $\mathrm{Tr}(Q_f) \notin \bar{\mathbb{Q}}_p$. We first need some definitions.

Definition 5.13. *(i) We define C_1 to be the set of f-tuples $(P_1, P_2, ..., P_f)$ where the types of the matrices P_i are chosen as follows: $P_1 \in \{t_2, t_3\}$. For $i = 2, 3, ..., f-1$, $P_i \in \{t_2, t_3\}$ if an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, and $P_i \in \{t_1, t_4\}$ if an odd number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type. Finally, $P_0 = t_3$ if an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, and $P_0 = t_4$ otherwise.*

(ii) We define C_2 to be the set of f-tuples $(P_1, P_2, ..., P_f)$ where the types of the matrices P_i are chosen as follows: $P_1 \in \{t_1, t_4\}$. For $i = 2, 3, ..., f-1$, $P_i \in \{t_1, t_4\}$ if an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, and $P_i \in \{t_2, t_3\}$ if an odd number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type. Finally, $P_0 = t_1$ if an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, and $P_0 = t_2$ otherwise.

In Definition 5.13 the type of the matrix P_0 has been chosen so that an even number of coordinates of the f-tuple $(P_1, P_2, ..., P_{f-1}, P_0)$ is of even type.

Definition 5.14. *(i) We define C_1^* to be the set of f-tuples $(P_1, P_2, ..., P_f)$ where the types of the matrices P_i are chosen as follows: $P_1 \in \{t_2, t_3\}$. For $i = 2, 3, ..., f-1$, $P_i \in \{t_2, t_3\}$ if an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, and $P_i \in \{t_1, t_4\}$ if an odd number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type. Finally, $P_0 = t_2$ if an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, and $P_0 = t_1$ otherwise.*

(ii) We define C_2^* to be the set of f-tuples $(P_1, P_2, ..., P_f)$ where the types of the matrices P_i are chosen as follows: $P_1 \in \{t_1, t_4\}$. For $i = 2, 3, ..., f-1$, $P_i \in \{t_1, t_4\}$ if an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, and $P_i \in \{t_2, t_3\}$ if an odd number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type. Finally, $P_0 = t_4$ if an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, and $P_0 = t_3$ otherwise.

In Definition 5.14 the type of the matrix P_0 has been chosen so that an odd number of coordinates of the f-tuple $(P_1, P_2, ..., P_{f-1}, P_0)$ is of even type.

Lemma 5.15. *Assume that $f \geq 2$ and, as before, let $Q_f = P_1 P_2 \cdots P_f$.*

(i) If $(P_1, P_2, ..., P_f) \in C_1^*$, then $Q_f = \begin{pmatrix} \alpha & \beta \\ \gamma & 0 \end{pmatrix}$ with β, γ nonconstant polynomials in $X_1, X_2, ..., X_f$ (with $X_f = X_0$), linearly independent over $\bar{\mathbb{Q}}_p$, and α nonscalar.

(ii) If $(P_1, P_2, ..., P_f) \in C_2^*$, then $Q_f = \begin{pmatrix} 0 & \beta \\ \gamma & \delta \end{pmatrix}$ with β, γ nonconstant polynomials in $X_1, X_2, ..., X_f$, linearly independent over $\bar{\mathbb{Q}}_p$, and δ nonscalar.

(iii) *If* $(P_1, P_2, ..., P_f) \in C_1$, *then* $Q_f = \begin{pmatrix} \alpha & \beta \\ 0 & \delta \end{pmatrix}$ *with* β *a nonzero polynomial in* $X_1, X_2, ..., X_f$, *and* α, δ *nonzero scalars.*

(iv) *If* $(P_1, P_2, ..., P_f) \in C_2$, *then* $Q_f = \begin{pmatrix} \alpha & 0 \\ \gamma & \delta \end{pmatrix}$ *with* γ *a nonzero polynomial in* $X_1, X_2, ..., X_f$, *and* α, δ *nonzero scalars.*

Proof. Follows easily by induction on f. □

Lemma 5.16. *Assume that* $f \geq 2$.

(i) *If an odd number of coordinates of* $(P_1, P_2, ..., P_f)$ *is of even type, then* Q_f *has one of the following forms:*

  (a) $Q_f = \begin{pmatrix} 0 & \beta \\ \gamma & \delta \end{pmatrix}$ *with* β, γ *nonconstant polynomials in* $X_1, X_2, ..., X_f$, *linearly independent over* $\bar{\mathbb{Q}}_p$, *and* δ *nonscalar. This case occurs if and only if* $(P_1, P_2, ..., P_f) \in C_2^*$.

  (b) $Q_f = \begin{pmatrix} \alpha & \beta \\ \gamma & 0 \end{pmatrix}$ *with* β, γ *nonconstant polynomials in* $X_1, X_2, ..., X_f$, *linearly independent over* $\bar{\mathbb{Q}}_p$, *and* α *nonscalar. This case occurs if and only if* $(P_1, P_2, ..., P_f) \in C_1^*$.

  (c) *In any other case,* $Q_f = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ *with* β, γ *nonconstant polynomials in* $X_1, X_2, ..., X_f$, *linearly independent over* $\bar{\mathbb{Q}}_p$, $\alpha\delta \neq 0$, *and* $\mathrm{Tr}\,(Q_f)$ *nonscalar.*

(ii) *If an even number of coordinates of* $(P_1, P_2, ..., P_f)$ *is of even type, then* Q_f *has one of the following forms:*

  (d) $Q_f = \begin{pmatrix} \alpha & \beta \\ 0 & \delta \end{pmatrix}$ *with* β *a nonzero polynomial in* $X_1, X_2, ..., X_f$, *and* α, δ *nonzero scalars. This case occurs if and only if* $(P_1, P_2, ..., P_f) \in C_1$.

  (e) $Q_f = \begin{pmatrix} \alpha & 0 \\ \gamma & \delta \end{pmatrix}$ *with* γ *a nonzero polynomial in* $X_1, X_2, ..., X_f$, *and* α, δ *nonzero scalars. This case occurs if and only if* $(P_1, P_2, ..., P_f) \in C_2$.

  (f) *In any other case,* $Q_f = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ *with* β, γ *nonconstant polynomials in* $X_1, X_2, ..., X_f$, *linearly independent over* $\bar{\mathbb{Q}}_p$, $\alpha\gamma \neq 0$ *and* $\mathrm{Tr}\,(Q_f)$ *is nonscalar.*

Proof. By induction on f. If $f=2$ the proof of the lemma is by a direct computation. Suppose $f\geq 3$. Case (i). An odd number of coordinates of $(P_1,P_2,...,P_f)$ is of even type.
(a) If an odd number of coordinates of $(P_1,P_2,...,P_{f-1})$ is of even type, then $P_0\in\{t_1,t_3\}$. We have the following three subcases:
(α) $Q_{f-1}=\begin{pmatrix}0&\beta\\ \gamma&\delta\end{pmatrix}$ with β,γ nonconstant polynomials in $X_1,X_2,,,.X_{f-1}$, linearly independent over $\bar{\mathbb{Q}}_p$, and δ nonscalar. If $P_0=t_1$, then Q_f is as in case (c), and by Lemma 5.15 $(P_1,P_2,...,P_f)\notin C_1^*\cup C_2^*$. If $P_0=t_3$, then Q_f is as in case (a). By the inductive hypothesis $(P_1,P_2,...,P_{f-1})\in C_2^*$, and since $P_0=t_3$, $(P_1,P_2,...,P_f)\in C_2^*$.
(β) $Q_{f-1}=\begin{pmatrix}\alpha&\beta\\ \gamma&0\end{pmatrix}$ with β,γ nonconstant polynomials in $X_1,X_2,,,.X_{f-1}$, linearly independent over $\bar{\mathbb{Q}}_p$, and α nonscalar. If $P_0=t_1$, then Q_f is as in case (b). By the inductive hypothesis $(P_1,P_2,...,P_{f-1})\in C_1^*$, and since $P_0=t_1$, $(P_1,P_2,...,P_f)\in C_1^*$. If $P_0=t_3$, then Q_f is as in case (c), and by Lemma 5.15 $(P_1,P_2,...,P_f)\notin C_1^*\cup C_2^*$.
(γ) $Q_{f-1}=\begin{pmatrix}\alpha&\beta\\ \gamma&\delta\end{pmatrix}$ with β,γ nonconstant polynomials in $X_1,X_2,,,.X_{f-1}$, linearly independent over $\bar{\mathbb{Q}}_p$, $\alpha\delta\neq 0$, and $\mathrm{Tr}\,(Q_f)$ nonscalar. If $P_0\in\{t_1,t_3\}$ then Q_f is as in case (c), and by Lemma 5.15 $(P_1,P_2,...,P_f)\notin C_1^*\cup C_2^*$.
(b) If an even number of coordinates of $(P_1,P_2,...,P_{f-1})$ is of even type, then $P_0\in\{t_2,t_4\}$. We have the following three subcases:
(α) $Q_{f-1}=\begin{pmatrix}\alpha&\beta\\ 0&\delta\end{pmatrix}$ with β a nonzero polynomial in $X_1,X_2,,,.X_{f-1}$, and α,δ nonzero scalars. If $P_0=t_2$, then Q_f is as in case (b). Since $(P_1,P_2,...,P_{f-1})\in C_1$ and $P_0=t_2$, $(P_1,P_2,...,P_f)\in C_1^*$. If $P_0=t_4$, then Q_f is as in case (c), and by Lemma 5.15 $(P_1,P_2,...,P_f)\notin C_1^*\cup C_2^*$.
(β) $Q_{f-1}=\begin{pmatrix}\alpha&0\\ \gamma&\delta\end{pmatrix}$ with γ a nonzero polynomial in $X_1,X_2,,,.X_{f-1}$, and α,δ nonzero scalars. If $P_0=t_2$, then Q_f is as in case (c), and by Lemma 5.15 $(P_1,P_2,...,P_f)\notin C_1^*\cup C_2^*$. If $P_0=t_4$, then Q_f is as in case (a). Since $(P_1,P_2,...,P_{f-1})\in C_2$ and $P_0=t_4$, $(P_1,P_2,...,P_f)\in C_2^*$.
(γ) $Q_{f-1}=\begin{pmatrix}\alpha&\beta\\ \gamma&\delta\end{pmatrix}$ with β,γ nonconstant polynomials in $X_1,X_2,,,.X_f$, linearly independent over $\bar{\mathbb{Q}}_p$, $\alpha\gamma\neq 0$ and $\mathrm{Tr}\,(Q_f)$ is nonscalar. Then $(P_1,P_2,...,P_{f-1})\notin C_1\cup C_2$. If $P_0\in\{t_2,t_4\}$, then Q_f is as in case (c), and by Lemma 5.15 $(P_1,P_2,...,P_f)\notin C_1^*\cup C_2^*$.
Case (ii). An even number of coordinates of $(P_1,P_2,...,P_f)$ is of even type. The rest of the lemma is proved by a case-by-case analysis similar to that of Case (i). □

Corollary 5.17. $\mathrm{Tr}\,(Q_f)\in\bar{\mathbb{Q}}_p$ *if and only if* $(P_1,P_2,...,P_{f-1},P_0)\in C_1\cup C_2$.

Remark 5.18. *If* $(P_1,P_2,...,P_f)\in C_1\cup C_2$*, the filtered* φ*-modules* $\mathbb{D}_{\vec{k}}^{\vec{i}}\,(\vec{0})$

are weakly admissible and the corresponding crystalline representation is split-reducible and ordinary (see §6.3). The filtered φ-modules $\mathbb{D}_{\vec{k}}^{\vec{i}}\ (\vec{\alpha})$ *make sense for any* $\vec{\alpha} \in \mathcal{O}_E^f$*. One can check by induction that* $\mathrm{Tr}\left(\varphi^f\right) = 1 + p^{\sum_{i=0}^{f-1} k_i}$*, therefore whenever* $\mathbb{D}_{\vec{k}}^{\vec{i}}\ (\vec{\alpha})$ *is weakly admissible the corresponding crystalline representation is reducible (see Proposition 6.5). Since we have not constructed the Wach modules which give rise to these filtered modules, weak admissibility is not automatic and has to be checked.*

We now turn our attention to condition (iv) of Lemma 4.4. By Proposition 5.1 the problematic cases are those with $\ell = k$, all the weights k_i equal and $Q_f \in \{E_{11}, E_{22}\}$. We have the following.

Lemma 5.19. *If* $\bar{Q}_f = E_{11}$ *then* $(P_1, ..., P_f) \in C_1$*; (ii) If* $\bar{Q}_f = E_{22}$*, then* $(P_1, ..., P_f) \in C_2$.

Proof. By induction on f. First, we notice that

$$P \mathrm{mod}\ (p \cdot Id,\ X_i \cdot Id) = \begin{cases} E_{22} \text{ if } P = t_1, \\ E_{12} \text{ if } P = t_2, \\ E_{11} \text{ if } P = t_3, \\ E_{21} \text{ if } P = t_4. \end{cases}$$

Suppose that $\bar{Q}_f = E_{11}$ and $f = 2$. Then $P_1 \in \{t_2, t_3\}$. If $P_1 = t_2$ then $P_0 = t_4$ and if $P_1 = t_3$ then $P_0 = t_3$. Suppose $\bar{Q}_f = E_{11}$ and $f > 2$. Then $\bar{Q}_{f-1} = E_{11}$ and $P_f = t_3$ or $\bar{Q}_{f-1} = E_{12}$ and $P_f = t_4$. In the first case the inductive hypothesis implies that $(P_1, P_2, ..., P_{f-1}) \in C_1$ and $P_f = t_3$. If an even number of coordinates of $(P_1, P_2, ..., P_{f-2})$ is of even type, then $P_{f-1} = t_3$. In this case an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type and $P_f = t_3$, hence $(P_1, ..., P_f) \in C_1$. If an odd number of coordinates of $(P_1, P_2, ..., P_{f-2})$ is of even type, then $P_{f-1} = t_4$. In this case an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type and $P_f = t_3$, hence $(P_1, ..., P_f) \in C_1$. Now assume that $\bar{Q}_{f-1} = E_{12}$ and $P_f = t_4$. This implies that either $\bar{Q}_{f-2} = E_{12}$, $P_{f-1} = t_4$ and $P_f = t_4$ which is absurd since in this case $\bar{Q}_f = 0$, or $\bar{Q}_{f-2} = E_{11}$, $P_{f-1} = t_2$ and $P_f = t_4$. If $f = 3$, then $P_1 = t_3$, $P_2 = t_2$, $P_3 = t_4$ and the lemma holds. If $f \geq 4$ and an even number of coordinates $(P_1, P_2, ..., P_{f-3})$ is of even type, then $P_{f-2} = t_3$, $P_{f-1} = t_2$ and $P_f = t_4$. Then an odd number of coordinates $(P_1, P_2, ..., P_{f-1})$ is of even type and $P_f = t_4$, hence $(P_1, ..., P_f) \in C_1$. If an odd number of coordinates $(P_1, P_2, ..., P_{f-3})$ is of even type, then $P_{f-2} = t_4$, $P_{f-1} = t_2$ and $P_f = t_4$. Then an odd number of coordinates $(P_1, P_2, ..., P_{f-1})$ is of even type and $P_f = t_4$, hence $(P_1, ..., P_f) \in C_1$. Part (ii) is proved similarly. □

Corollary 5.20. *If* $(P_1, P_2, ..., P_f) \in \mathcal{P}$ *and* $\mathrm{Tr}\,(Q_f) \notin \bar{\mathbb{Q}}_p$*, then the operator*

$$\overline{H} \mapsto \overline{H - Q_f H(p^{f\ell} Q_f^{-1})} : \widetilde{M}_2 \to \widetilde{M}_2$$

is surjective.

5.2 Corresponding families of rank two filtered φ-modules

Let $\Pi^{\vec{i}}(\mathcal{S}) = (\Pi_1(X_1), \Pi_2(X_2), ..., \Pi_{f-1}(X_{f-1}), \Pi_0(X_0))$ with $\vec{i} \in \{1,2,3,4\}^f$ and matrices $\Pi_i(X_i)$ as in Definition 5.4. The definition of the Π_i and $P_i = \Pi_i \mathrm{mod}\ \pi$ depends on the choice of the z_i in Proposition 5.9 and therefore on ℓ. For the rest of the paper we assume that $(P_1, P_2, ..., P_0) \notin C_1 \cup C_2$ and we choose $\ell = k = \max\{k_0, k_1, ..., k_{f-1}\}$.

Proposition 5.21. *For any $\gamma \in \Gamma_K$, there exists a unique matrix $G_\gamma(\mathcal{S}) = G_\gamma(\mathcal{S}) \in M_2^{\mathcal{S}}$ such that:*

(i) $G_\gamma(\mathcal{S}) \equiv \overrightarrow{Id} \mathrm{mod}\ \vec{\pi}$;

(ii) $\Pi^{\vec{i}}(\mathcal{S})\varphi(G_\gamma(\mathcal{S})) = G_\gamma(\mathcal{S})\gamma(\Pi^{\vec{i}}(\mathcal{S}))$.

Proof. Conditions (1) and (2) of Lemma 4.4 are satisfied by Proposition 5.9. Condition (3) of Lemma 4.4 is satisfied by the assumption that $(P_1, P_2, ..., P_0) \notin C_1 \cup C_2$ and Corollaries 5.3 and 5.17. Finally, condition (4) of Lemma 4.4 is satisfied by Proposition 5.1 and Lemma 5.19. The proposition follows from Lemma 4.4. ☐

For any $\vec{a} \in \mathfrak{m}_E^f$ we equip the module $\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}) = \left(\mathcal{O}_E[[\pi]]^{|\tau|}\right)\eta_1 \bigoplus \left(\mathcal{O}_E[[\pi]]^{|\tau|}\right)\eta_2$ with semilinear φ and Γ_K-actions defined as in Proposition 4.6. For any $\vec{a} \in \mathfrak{m}_E^f$ we consider the matrices of $\mathrm{GL}_2\left(E^{|\tau|}\right)$ obtained from the matrices $P^{\vec{i}}(\vec{a}) = (P_1(X_1), P_2(X_2), ..., P_{f-1}(X_{f-1}), P_0(X_0))$ by substituting $X_j = a_j$ in $P_j(X_j)$. We define families of filtered φ-modules $\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{a}) = \left(E^{|\tau|}\right)\eta_1 \bigoplus \left(E^{|\tau|}\right)\eta_2$ with Frobenius endomorphisms given by $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2)P^{\vec{i}}(\vec{a})$, and filtrations given by

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{a})) = \begin{cases} E^{|\tau|}\eta_1 \bigoplus E^{|\tau|}\eta_2 & \text{if } j \leq 0, \\ E^{|\tau_{I_0}|}\left(\vec{x}\eta_1 + \vec{y}\eta_2\right) & \text{if } 1 \leq j \leq w_0, \\ E^{|\tau_{I_1}|}\left(\vec{x}\eta_1 + \vec{y}\eta_2\right) & \text{if } 1 + w_0 \leq j \leq w_1, \\ \quad\cdots\cdots & \\ E^{|\tau_{I_{t-1}}|}\left(\vec{x}\eta_1 + \vec{y}\eta_2\right) & \text{if } 1 + w_{t-2} \leq j \leq w_{t-1}, \\ \quad 0 & \text{if } j \geq 1 + w_{t-1}, \end{cases} \tag{5.10}$$

where $\vec{x} = (x_0, x_1, ..., x_{f-1})$ and $\vec{y} = (y_0, y_1, ..., y_{f-1})$ with

$$(x_i, y_i) = \begin{cases} (1, -\alpha_i) & \text{if } P_i \text{ has type 1 or 2}, \\ (-\alpha_i, 1) & \text{if } P_i \text{ has type 3 or 4}, \end{cases} \tag{5.11}$$

and $\alpha_i = a_i z_i(0)$ for all i. Since $\ell = k$, Remark 5.12 implies that $\alpha_i \in p^m \mathfrak{m}_E$ for all i, where

$$m := \begin{cases} \lfloor \frac{k-1}{p-1} \rfloor & \text{if } k \geq p \text{ and } k_i \neq p \text{ for some } i, \\ 0 & \text{if } k \leq p-1 \text{ or } k_i = p \text{ for all } i. \end{cases}$$

Proposition 5.22. *For any* $\vec{a} \in \mathfrak{m}_E^f$ *the filtered* φ*-modules* $(\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{a}), \varphi)$ *defined above are weakly admissible and* $\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{a}) \simeq E^{|\tau|} \bigotimes_{\mathcal{O}_E^{|\tau|}} (\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}))$ *as filtered* φ*-modules over* $E^{|\tau|}$.

Proof. By Theorem 2.4, $\vec{x}\eta_1 + \vec{y}\eta_2 \in \mathrm{Fil}^{\mathrm{j}}(\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}))$ if and only if $\varphi(\vec{x})\varphi(\eta_1) + \varphi(\vec{y})\varphi(\eta_2) \in q^j \mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})$ or equivalently

$$e_i\varphi(\vec{x})\varphi(\eta_1) + e_i\varphi(\vec{y})\varphi(\eta_2) \in q^j e_i\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}) \text{ for all } i \in I_0, \tag{5.12}$$

with the idempotents e_i as in §1.1. We fix some $i \in I_0$ and calculate in the case where Π_i is of type 2. Then $\Pi_i(a_i) = \begin{pmatrix} 0 & c_i q^{k_i} \\ 1 & a_i\varphi(z_i) \end{pmatrix}$ and equation 5.12 is equivalent to $\begin{cases} q^j \mid \varphi(y_i)q^{k_i}, \\ q^j \mid \varphi(x_i + y_i a_i z_i). \end{cases}$ We use that $q^j \mid \varphi(x)$ if and only if $\pi^j \mid x$ for any $x \in \mathcal{O}_E[[\pi]]$. If $j \geq 1 + k_i$, then $x_i, y_i \equiv 0 \mathrm{mod}\ \pi$. If $1 \leq j \leq k_i$, the system above is equivalent to $\pi^j \mid x_i + y_i a_i z_i$. Since $a_i z_i \equiv \alpha_i \mathrm{mod}\ \pi$,

$$e_i\vec{x}\eta_1 + e_i\vec{y}\eta_2 + \pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}) = \begin{cases} \alpha_i\bar{y}_i e_i\eta_1 + \bar{y}_i e_i\eta_2 + \pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}) & \text{if } 1 \leq j \leq k_i, \\ 0 & \text{if } j \geq k_i \end{cases}$$

where $\bar{y}_i = y_i \mathrm{mod}\ \pi$ can be any element of $\mathcal{O}_E$. Since $\mathrm{Fil}^0(\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})) = (\mathcal{O}_E^{|\tau|})\eta_1 \bigoplus (\mathcal{O}_E^{|\tau|})\eta_2$, we get

$$e_i\mathrm{Fil}^{\mathrm{j}}(\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})) = \begin{cases} e_i(\mathcal{O}_E^{|\tau|})\eta_1 \bigoplus e_i(\mathcal{O}_E^{|\tau|})\eta_2 & \text{if } j \leq 0, \\ e_i(\mathcal{O}_E^{|\tau|})(\vec{x}^i\eta_1 + \vec{y}^i\eta_2) & \text{if } 1 \leq j \leq k_i, \\ 0 & \text{if } j \geq 1 + k_i, \end{cases}$$

with $e_i\vec{x}^i = (0, ..., x_i, ..., 0)$, $e_i\vec{y}^i = (0, ..., y_i, ..., 0)$ and $(x_i, y_i) = (-\alpha_i, 1)$. Calculating for the other choices of $\Pi_i(a_i)$ we see that for all $i \in I_0$, (x_i, y_i) is as in formula 5.10. Since $\mathrm{Fil}^{\mathrm{j}}(\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})) = \bigoplus_{i=0}^{f-1} e_i\mathrm{Fil}^{\mathrm{j}}(\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}))$, arguing as in the proof of Proposition 3.4 we get

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})) = \begin{cases} (\mathcal{O}_E^{|\tau|})\eta_1 \bigoplus (\mathcal{O}_E^{|\tau|})\eta_2 & \text{if } j \leq 0, \\ (\mathcal{O}_E^{|\tau|})f_{I_0}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } 1 \leq j \leq w_0, \\ (\mathcal{O}_E^{|\tau|})f_{I_1}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } 1 + w_0 \leq j \leq w_1, \\ \cdots\cdots & \\ (\mathcal{O}_E^{|\tau|})f_{I_{t-1}}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } 1 + w_{t-2} \leq j \leq w_{t-1}, \\ 0 & \text{if } j \geq 1 + w_{t-1}, \end{cases}$$

with $\vec{x} = (x_0, x_1, ..., x_{f-1})$ and $\vec{y} = (y_0, y_1, ..., y_{f-1})$ and (x_i, y_i) as in formula 5.10. The isomorphism $\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{a}) \simeq E^{|\tau|} \bigotimes_{\mathcal{O}_E^{|\tau|}} (\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a})/\pi\mathbb{N}_{\vec{k}}^{\vec{i}}(\vec{a}))$ is now obvious. □

The crystalline representation corresponding to $\mathbb{D}_{\vec{k}}^{\vec{i}}(\vec{a})$ is denoted by $V_{\vec{k},\vec{a}}^{\vec{i}}$.

6 Reductions of crystalline representations

In this section we explicitly compute the semisimplified modulo p reductions of the families of crystalline representations constructed in §5. We will need the following lemma.

Lemma 6.1. *Let F be any field, G any group and H any finite index subgroup. Let V be an irreducible finite-dimensional FG-module whose restriction to H contains some FH-submodule W with $\dim_F V = [G:H]\dim_F W$. Then $V \simeq \mathrm{Ind}_H^G(W)$.*

Proof. By Frobenius reciprocity there exists some nonzero $\alpha \in \mathrm{Hom}_{FG}(\mathrm{Ind}_H^G(W), V)$. It is an isomorphism because V is irreducible and $\mathrm{Ind}_H^G(W)$ and V have the same dimension over F. □

We start with the reductions of crystalline characters and reducible two-dimensional crystalline representations of G_K. The embeddings τ_i of K_f into E fixed in the introduction induce embeddings of residue fields $k_{K_f} \xrightarrow{\bar{\tau}_i} k_E$. The level f fundamental characters $\omega_{f,\bar{\tau}_i}$ of I_{K_f} are defined by composing the embeddings $\bar{\tau}_i$ with the homomorphism $I_{K_f} \to k_{K_f}^{\times}$ obtained from local class field theory, with uniformizers corresponding to geometric Frobenius elements. We recall the following lemma which follows immediately from [BDJ, Lemma 3.8], where the χ_i are as in §3.

Lemma 6.2. *(i) $(\bar{\chi}_i)_{|I_{K_f}} = \omega_{f,\bar{\tau}_{i+1}}^{-1}$ for $i = 0,1,...,f-1$; (ii) $\omega_{f,\bar{\tau}_i} = \omega_{f,\bar{\tau}_0}^{p^i}$ for all i; (iii) $\omega_{2f,\bar{\tau}_0}^{1+p^f} = \omega_{f,\bar{\tau}_0}$; (iv) $\omega = \prod\limits_{i\in I_0} \omega_{f,\bar{\tau}_i}$, where ω is the cyclotomic character modulo $\mathfrak{m}_E$.*

Our next goal is to compute the determinant of a two-dimensional crystalline representations in terms of its labeled Hodge-Tate weights. To do this, we will need some facts about weakly admissible filtered φ-modules which we briefly recall. For the missing details we refer to [Dou10]. We remark that similar results for odd p have been obtained by Imai in [Ima09].

Proposition 6.3. *Let $(\mathbb{D},\varphi)$ be a rank two F-semisimple, nonscalar filtered φ-module over $E^{|\tau|}$ with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$. After enlarging E if necessary, there exists an ordered basis $\underline{\eta}$ of $\mathbb{D}$ over $E^{|\tau|}$ with respect to which the matrix of Frobenius takes the form $\mathrm{Mat}_{\underline{\eta}}(\varphi) = \mathrm{diag}(\vec{\alpha},\vec{\delta})$ for some vectors $\vec{\alpha},\vec{\delta} \in (E^{\times})^{|\tau|}$ with $\mathrm{Nm}_{\varphi}(\vec{\alpha}) \neq \mathrm{Nm}_{\varphi}(\vec{\delta})$. The filtration in the same basis has the form of formula 5.10 for some vectors $\vec{x},\vec{y} \in E^{|\tau|}$ with $(x_i,y_i) \neq (0,0)$ for all $i \in I_0$. We call such a basis $\underline{\eta}$ a standard basis of $(\mathbb{D},\varphi)$. The Frobenius-fixed submodules are 0, $\mathbb{D}$, $\mathbb{D}_1 := \left(E^{|\tau|}\right)\eta_1$ and $\mathbb{D}_2 := \left(E^{|\tau|}\right)\eta_2$. The module $\mathbb{D}$*

is weakly admissible if and only if

$$(1)\ \mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\alpha})\mathrm{Nm}_\varphi(\vec{\delta})) = \sum_{i\in I_0} k_i;$$

$$(2)\ \mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\alpha})) \geq \sum_{\{i\in I_0:\ y_i=0\}} k_i;$$

$$(3)\ \mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\delta})) \geq \sum_{\{i\in I_0:\ x_i=0\}} k_i.$$

Assuming that $\mathbb{D}$ is weakly admissible,

(i) The filtered φ-module $\mathbb{D}$ is irreducible if and only if both the inequalities (2) *and* (3) *above are strict;*

(ii) The filtered φ-module $\mathbb{D}$ is split-reducible if and only if both inequalities (2) *and* (3) *are equalities, or equivalently $I_0^+ \cap J_{\vec{x}} \cap J_{\vec{y}} = \varnothing$. In this case, the only nontrivial weakly admissible submodules are $\mathbb{D}_i$, $i = 1, 2$, and we have $\mathbb{D} = \mathbb{D}_1 \bigoplus \mathbb{D}_2$;*

(iii) In any other case the filtered φ-module $\mathbb{D}$ is reducible, non-split.

In the Proposition above, if $\mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\alpha})) = \sum_{\{i\in I_0:\ y_i=0\}} k_i$, the only nontrivial weakly admissible submodule is $(\mathbb{D}_1, \varphi)$. If $\mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\delta})) = \sum_{\{i\in I_0:\ x_i=0\}} k_i$, the only nontrivial weakly admissible submodule is $(\mathbb{D}_2, \varphi)$. If $(\mathbb{D}, \varphi)$ is not F-semisimple, after extending E if necessary, there exists an ordered basis $\underline{\eta} = (\eta_1, \eta_2)$ of $\mathbb{D}$ over $E^{|\tau|}$ with respect to which the matrix of Frobenius takes the form

$$\mathrm{Mat}_{\underline{\eta}}(\varphi) = \begin{pmatrix} \vec{\alpha} & \vec{0} \\ \vec{\gamma} & \vec{\alpha} \end{pmatrix}$$

for some vectors $\vec{\alpha} \in (E^\times)^{|\tau|}$ and $\vec{\gamma} \in E$ (see [Dou10, §2.1]). The filtration in this basis has the shape of formula 5.10. The filtered φ-module $(\mathbb{D}, \varphi)$ is weakly admissible if any only if $2 \cdot \mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\alpha})) = \sum_{i\in I_0} k_i$ and $\mathrm{v_p}(\mathrm{Nm}_\varphi(\vec{\alpha})) \geq \sum_{\{i\in I_0:x_i=0\}} k_i$. The corresponding crystalline representation is irreducible if and only if the latter inequality is strict and reducible, non-split otherwise. In this case, the only φ-stable weakly admissible submodule is $(\mathbb{D}_2, \varphi)$ (see also [Dou10, § 5.4]). If $(\mathbb{D}, \varphi)$ is F-scalar, there exists an ordered basis $\underline{\eta} = (\eta_1, \eta_2)$ of $\mathbb{D}$ over $E^{|\tau|}$ with respect to which $\mathrm{Mat}_{\underline{\eta}}(\varphi) = \mathrm{diag}\left(\alpha \cdot \vec{1}, \alpha \cdot \vec{1}\right)$ for some $\alpha \in E^\times$ and the filtration is as in formula 5.10. The only φ-stable submodules are the $\mathbb{D}_i$, $i = 1, 2$ and $\mathbb{D}(c) = \left(E^{|\tau|}\right)(\eta_1 + c \cdot \vec{1} \cdot \eta_2)$ for any $c \in E^\times$ (cf. [Dou10, §5.3]). To summarize, we have the following.

Proposition 6.4. *Let $(\mathbb{D},\varphi)$ be a reducible weakly admissible rank two filtered φ-module over $E^{|\tau|}$ with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$. After enlarging E if necessary, there exists an ordered basis $\underline{\eta}=(\eta_1,\eta_2)$ of $\mathbb{D}$ over $E^{|\tau|}$ with respect to which the matrix of Frobenius takes the form $\mathrm{Mat}_{\underline{\eta}}(\varphi)=\begin{pmatrix}\vec{\alpha} & \vec{0}\\ * & \vec{\delta}\end{pmatrix}$ and is such that $\mathbb{D}_2=\left(E^{|\tau|}\right)\eta_2$ is a φ-stable, weakly admissible submodule.*

The following propositions which will be used in §§ 6.2 and 6.3.

Proposition 6.5. *A rank two weakly admissible effective filtered φ-module $(\mathbb{D},\varphi)$ with labeled Hodge-Tate weights $\{-k_i,0\}_{\tau_i}$ and $\mathrm{v_p}\left(\mathrm{Tr}(\varphi^f)\right)=0$ is reducible.*

Proof. If $\mathbb{D}$ is F-semisimple and nonscalar, see [Dou10, Corollary 7.2]. Suppose that this is not the case. Since we assume that $k_i>0$ for at least one i, for any F-scalar or non-F-semisimple filtered φ-module with labeled weights $\{-k_i,0\}_{\tau_i}$, $\mathrm{v_p}\left(\mathrm{Tr}(\varphi^f)\right)\neq 0$. Indeed, in this case there exists an ordered basis $\underline{\eta}$ of $\mathbb{D}$ over $E^{|\tau|}$ with respect to which the matrix of Frobenius takes the form

$$\mathrm{Mat}_{\underline{\eta}}(\varphi)=\begin{pmatrix}\vec{\alpha} & \vec{0}\\ \vec{\gamma} & \vec{\alpha}\end{pmatrix}$$

for some vectors $\vec{\alpha}\in(E^{\times})^{|\tau|}$ and $\vec{\gamma}\in E$ (see [Dou10, §2.1]). Weak admissibility implies that $2\cdot\mathrm{v_p}(\mathrm{Nm}_{\varphi}(\vec{\alpha}))=\sum_{i\in I_0}k_i>0$ (see [Dou10, Propositions 4.3 and 4.4]), therefore $\mathrm{v_p}\left(\mathrm{Tr}(\varphi^f)\right)=\mathrm{v_p}\left(2\cdot\mathrm{Nm}_{\varphi}(\vec{\alpha})\right)>0$. □

The following lemma allows us to compute determinants of two-dimensional crystalline representations in terms of their labeled Hodge-Tate weights.

Lemma 6.6. *If $(\mathbb{D},\varphi)$ is a rank two weakly admissible filtered φ-module over K with E-coefficients and labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$, then $(\wedge^2_{E\otimes K}\mathbb{D},\wedge^2_{E\otimes K}\varphi)$ is weakly admissible with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$.*

Proof. Let $\underline{\eta}=(\eta_1,\eta_2)$ be a standard basis of $(\mathbb{D},\varphi)$ such that $\mathrm{Mat}_{\underline{\eta}}(\varphi)$ is as in Proposition 6.4 and $\mathrm{Fil^j}\mathbb{D}$ as in Formula 5.10. Clearly $(\wedge^2\varphi)(\eta_1\wedge\eta_2)=\vec{\alpha}\cdot\vec{\delta}(\eta_1\wedge\eta_2)$. Since $\mathrm{Fil^j}(\mathbb{D}\wedge\mathbb{D})=\sum_{j_1+j_2=j}(\mathrm{Fil^{j_1}}\mathbb{D}\wedge_{E\otimes K}\mathrm{Fil^{j_2}}\mathbb{D})$ and $J_{\vec{x}}\cup J_{\vec{y}}=I_0$, a simple computation yields

$$\mathrm{Fil^j}(\mathbb{D}\wedge\mathbb{D})=\begin{cases} E^{|\tau_{I_0}|}(\eta_1\wedge\eta_2) & \text{if } j\leq w_0,\\ E^{|\tau_{I_1}|}(\eta_1\wedge\eta_2) & \text{if } 1+w_0\leq j\leq w_1,\\ \quad\cdots\cdots & \\ E^{|\tau_{I_{t-1}}|}(\eta_1\wedge\eta_2) & \text{if } 1+w_{t-2}\leq j\leq w_{t-1},\\ 0 & \text{if } j\geq 1+w_{t-1},\end{cases}$$

from which the statement about the labeled Hodge-Tate weights follows immediately. Weak admissibility is clear. □

Corollary 6.7. *If V is the crystalline representation corresponding to $\mathbb{D}$, then*

$$\det V \simeq \eta \cdot \chi_{e_0}^{k_1} \cdot \chi_{e_1}^{k_2} \cdot \cdots \cdot \chi_{e_{f-2}}^{k_{f-1}} \cdot \chi_{e_{f-1}}^{k_0} \text{ and } (\det \overline{V})_{|I_K} \simeq \omega_{f,\bar{\tau}_0}^{\alpha},$$

where η is an unramified character of G_K and $\alpha = -\sum_{i=0}^{f-1} p^i k_i$.

Proof. By Proposition 3.4 and Lemma 6.6 the crystalline character $\det V \otimes \left(\chi_{e_0}^{k_1} \cdot \chi_{e_1}^{k_2} \cdot \cdots \cdot \chi_{e_{f-2}}^{k_{f-1}} \cdot \chi_{e_{f-1}}^{k_0}\right)^{-1}$ has labeled Hodge-Tate weights $\{0\}_{\tau_i}$. If the corresponding filtered φ-module has Frobenius endomorphism $\varphi(\eta) = \vec{a}\cdot\eta$, then by Proposition 3.5 $\mathrm{Nm}_{\varphi}(\vec{a}) = c \cdot \vec{1}$ for some $c \in E^{\times}$ with $\mathrm{v_p}(c) = 0$. Lemma 3.7 implies that $\det V \otimes \left(\chi_{e_0}^{k_1} \cdot \chi_{e_1}^{k_2} \cdot \cdots \cdot \chi_{e_{f-2}}^{k_{f-1}} \cdot \chi_{e_{f-1}}^{k_0}\right)^{-1}$ is the unramified character of G_K which maps Frob_K to c. The rest of the corollary follows from Lemma 6.2. ∎

We recall the following well-known proposition in which the field K has absolute inertia degree f and is not assumed to be unramified over $\mathbb{Q}_p$.

Proposition 6.8. *[Bre07, Prop. 2.7] Let $\bar{\rho} : G_K \to \mathrm{GL}_2(\bar{\mathbb{F}}_p)$ be a continuous representation. Then*

$$\bar{\rho}_{|I_K} \simeq \begin{pmatrix} \omega_{2f}^{m} & * \\ 0 & \omega_{2f}^{mp^f} \end{pmatrix}$$

for some integer m. The representation $\bar{\rho}$ is irreducible if and only $1 + p^f \nmid m$, and in this case $* = 0$.

Corollary 6.9. *Let χ be a crystalline character of $G_{K_{2f}}$ with labeled Hodge-Tate weights $\{-k_i\}_{\tau_i}$, where the k_i are arbitrary integers for all $i = 0, 1, ..., 2f-1$, and let $V = \mathrm{Ind}_{K_{2f}}^{K_f}(\chi)$. The residual representation $\overline{V}$ is irreducible if and only if $1 + p^f \nmid \sum_{i=0}^{2f-1} p^i k_i$.*

Proof. Follows immediately from Lemma 6.2 and Proposition 6.8. ∎

6.1 Reductions of reducible two-dimensional crystalline representations

In this section we compute the semisimplified modulo p reduction of any reducible two-dimensional crystalline representation of G_{K_f}.

Lemma 6.10. *Let $k_0, k_1, ..., k_{f-1}$ be arbitrary integers and let*

$$\mathrm{Fil}^{\mathrm{j}}\mathbb{D} = \begin{cases} E^{|\tau_{I_0}|}\eta & \text{if } j \leq w_0, \\ E^{|\tau_{I_1}|}\eta & \text{if } \ 1 + w_0 \leq j \leq w_1, \\ \cdots\cdots & \\ E^{|\tau_{I_{t-1}}|}\eta & \text{if } 1 + w_{t-2} \leq j \leq w_{t-1}, \\ 0 & \text{if } j \geq 1 + w_{t-1}. \end{cases} \tag{6.1}$$

For each $i \in I_0$,

$$e_i\mathrm{Fil}^{\mathrm{j}}\mathbb{D} = \begin{cases} e_iE^{|\tau_{I_0}|}\eta & \text{if } j \leq k_i, \\ 0 & \text{if } r \geq 1 + k_i. \end{cases}$$

Proof. Let $k_i = w_r$ for some $r \in \{1, ..., t-1\}$. Since $w_r > w_{r-1}$ we have $i \in I_r$ from the definition of I_r. Similarly, since $k_i = w_r$ we have $i \notin I_{r+1}$. The same is clear for $r = 0$. Hence $e_i f_{I_r} = e_i$ and $e_i f_{I_{r+1}} = 0$ for all r. Multiplying formula 6.1 by e_i, we get

$$e_i\mathrm{Fil}^{\mathrm{j}}\mathbb{D} = \begin{cases} e_iE^{|\tau_{I_0}|}\eta & \text{if } j \leq w_r, \\ 0 & \text{if } r \geq 1 + w_r. \end{cases}$$

□

Let $\mathbb{D}$ be as in Proposition 6.4 and let $\mathrm{Mat}_{\underline{\eta}}(\varphi) = \begin{pmatrix} \vec{\alpha} & \vec{0} \\ * & \vec{\delta} \end{pmatrix}$. The filtration is as in formula 5.10 for some vectors $\vec{x}, \vec{y} \in E^{|\tau|}$. By Proposition 2.10 in [Dou10] (or by a direct computation),

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}_2) = \mathbb{D}_2 \cap \mathrm{Fil}^{\mathrm{j}}\mathbb{D} = \begin{cases} \mathbb{D}_2 & \text{if } \ j \leq 0, \\ E^{|\tau_{I_{0,\vec{x}}}|}\eta_2 & \text{if } \ 1 \leq j \leq w_0, \\ \cdots\cdots & \\ E^{|\tau_{I_{t-1,\vec{x}}}|}\eta_2 & \text{if } \ 1 + w_{t-2} \leq j \leq w_{t-1}, \\ 0 & \text{if } \ j \geq 1 + w_{t-1}, \end{cases}$$

where $I_{r,\vec{x}} = I_r \cap J'_{\vec{x}} = \{i \in I_r : x_i = 0\}$. Let $\vec{\delta} = (\delta_0, \delta_1, ..., \delta_{f-1})$. By Lemma 6.10,

$$e_i\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}_2) = \begin{cases} e_iE^{|\tau|}\eta_2 & \text{if } j \leq 0 \\ e_iE^{|\tau|}f_{J'_{\vec{x}}}\eta_2 & \text{if } 1 \leq j \leq k_i, \\ 0 & \text{if } j \geq 1 + k_i, \end{cases}$$

therefore the labeled Hodge-Tate weight of $\mathbb{D}_2$ with respect to the embedding τ_i is

$$m_i = \begin{cases} 0 & \text{if } x_i \neq 0 \ , \\ k_i & \text{if } x_i = 0, \end{cases}$$

and $(\mathbb{D}_2, \varphi_2)$ corresponds to the effective crystalline character $\chi_{c,\vec{0}} \cdot \chi_{e_{f-1}}^{m_0} \cdot \chi_{e_0}^{m_1} \cdot \cdots \cdot \chi_{e_{f-2}}^{m_{f-1}}$, where $c = \left(\prod_{i \in I_0} \delta_i\right) \cdot p^{-\sum_{i \in I_0} k_i}$. The following theorem follows immediately from Corollary 6.7.

THEOREM 6.11. *(i)*

$$V \simeq \begin{pmatrix} \psi_1 & * \\ 0 & \psi_2 \end{pmatrix},$$

where $\psi_1 = \eta_1 \cdot \chi_{e_{f-1}}^{m_0} \cdot \chi_{e_0}^{m_1} \cdot \cdots \cdot \chi_{e_{f-2}}^{m_{f-1}}$ *and* $\psi_2 = \eta_2 \cdot \chi_{e_0}^{k_1 - m_1} \cdot \chi_{e_1}^{k_2 - m_2} \cdot \cdots \cdot \chi_{e_{f-2}}^{k_{f-1} - m_{f-1}} \cdot \chi_{e_{f-1}}^{k_0 - m_0}$, *where* η_i *are unramified characters of* G_{K_f}.

(ii)

$$\left(\overline{V}_{|I_K}\right)^{s.s.} = \omega_{f,\bar{\tau}_0}^{\alpha_1} \oplus \omega_{f,\bar{\tau}_0}^{\alpha_2},$$

where $\alpha_1 = -\sum_{i=0}^{f-1} m_i p^i$ *and* $\alpha_2 = \sum_{i=0}^{f-1} (m_i - k_i)\, p^i$.

Notice that for an ordered basis is in Proposition 6.4, $\left(\overline{V}_{|I_{K_f}}\right)^{s.s.}$ only depends on the filtration with respect to that basis.

6.2 Proof of theorem 1.5

Let $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$ for $i = 0, 1, ..., f-1$ and assume that at least one k_i is strictly positive. In this section we construct infinite families of crystalline representations of Hodge-Tate type $\{0, -k_i\}_{\tau_i}$ which contain the irreducible representations $V_{\vec{\ell}} = \mathrm{Ind}_{G_{K_{2f}}}^{G_{K_f}} \left(\chi_{e_0}^{\ell_1} \cdot \chi_{e_1}^{\ell_2} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}} \cdot \chi_{e_{2f-1}}^{\ell_0} \right)$ of Proposition 3.11, and have the same mod p reductions with $V_{\vec{\ell}}$. We choose f-tuples of matrices $(\Pi_1, \Pi_2, ..., \Pi_f)$ (with $\Pi_f = \Pi_0$), where the types of the matrices Π_i (recall Definition 5.4) are chosen as follows:
(1) If $\ell_1 = 0$, $\Pi_1 \in \{t_2, t_3\}$;
(2) If $\ell_1 = k_1 > 0$, $\Pi_1 \in \{t_1, t_4\}$.
For $i = 2, 3, ..., f-1$, we choose the type of the matrix Π_i as follows:
(1) If $\ell_i = 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{i-1})$ is of even type, $\Pi_i \in \{t_2, t_3\}$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{i-1})$ is of even type, $\Pi_i \in \{t_1, t_4\}$.

(2) If $\ell_i = k_i > 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{i-1})$ is of even type, $\Pi_i \in \{t_1, t_4\}$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{i-1})$ is of even type, $\Pi_i \in \{t_2, t_3\}$.

Finally, we choose the type of the matrix Π_0 as follows:
(1) If $\ell_0 = 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_4$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_3$.

(2) If $\ell_0 = k_0 > 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_2$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_1$.

Notice that from the choice of Π_0, an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_f)$ is of even type. Let $\vec{i} = (i_1, i_2, ..., i_0) \in \{1,2,3,4\}^f$ be the type-vector attached to $(\Pi_1, \Pi_2, ..., \Pi_f)$. For the matrices Π_i, we assume that $c_i = 1$ for all i. Let $P_i = \Pi_i \bmod \pi$ for each i and notice that from the choice of the matrices Π_i it follows that $(P_1, P_2, ..., P_f) \notin C_1 \cup C_2$. The type of P_i is defined to be the type of Π_i. For any $\vec{a} \in \mathfrak{m}_E^f$ we consider the families of crystalline E-representations $V_{\vec{k}}^{\vec{i}}(\vec{a})$ of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$ constructed in §5.2. We prove the following.

Proposition 6.12. *(i)* $V_{\vec{k}}^{\vec{i}}(\vec{0}) = \mathrm{Ind}_{K_{2f}}^{K_f}\left(\chi_{e_0}^{\ell_1} \cdot \chi_{e_1}^{\ell_2} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}} \cdot \chi_{e_{2f-1}}^{\ell_0}\right)$ *and* $V_{\vec{k}}^{\vec{i}}(\vec{0})$ *is irreducible;*

(ii) For any $\vec{a} \in \mathfrak{m}_E^f$, $\overline{V}_{\vec{k}}^{\vec{i}}(\vec{a}) = \overline{V}_{\vec{k}}^{\vec{i}}(\vec{0})$;

(iii) For any $\vec{a} \in \mathfrak{m}_E^f$, $\left(\overline{V}_{\vec{k}}^{\vec{i}}(\vec{a})_{|I_{K_f}}\right)^{s.s.} = \omega_{2f,\bar{\tau}_0}^{\beta} \bigoplus \omega_{2f,\bar{\tau}_0}^{p^f\beta}$, *where* $\beta = -\sum_{i=0}^{2f-1} p^i \ell_i$;

(iv) $\overline{V}_{\vec{k}}^{\vec{i}}(\vec{a})$ *is irreducible if and only if* $1 + p^f \nmid \beta$;

(v) Any irreducible member of the family $\left\{V_{\vec{k}}^{\vec{i}}(\vec{a}),\ \vec{a} \in \mathfrak{m}_E^f\right\}$, *other than* $V_{\vec{k}}^{\vec{i}}(\vec{0})$, *is non-induced.*

Proof. We restrict $V_{\vec{k}}^{\vec{i}}(\vec{0})$ to $G_{K_{2f}}$. By the construction of the representation $V_{\vec{k}}^{\vec{i}}(\vec{0})$ in §5.1, there exists some G_{K_f}-stable lattice $\left(\mathrm{T}_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{G_{K_f}}$ inside $V_{\vec{k}}^{\vec{i}}(\vec{0})$ whose Wach module has φ-action defined by $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2)\,\Pi(\vec{0})$, where $\Pi(\vec{0}) = (\Pi_1(0), \Pi_2(0), ..., \Pi_{f-1}(0), \Pi_0(0))$. By Proposition 2.6, the Wach module of the $G_{K_{2f}}$-stable lattice $\left(\mathrm{T}_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ inside $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ is defined by $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2)\,\Pi(0)^{\otimes 2}$, therefore the filtered φ-module corresponding to $\left(V_{\vec{k},\vec{0}}^{\vec{i}}\right)_{|G_{K_{2f}}}$ has Frobenius endomorphism $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2)\,P(\vec{0})^{\otimes 2}$. By Corollary 2.7 the restricted representation $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ has labeled Hodge-Tate weights $(\{0, -k_i\})_{\tau_i}$, $i =$

$0,1,...,2f-1$, with $k_{i+f}=k_i$ for $i=0,1,...,f-1$, and filtration as in formula 5.10 for some vectors $\vec{x},\vec{y}$, with the sets I_j being defined with respect to the $2f$ weights above. We prove that $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ is reducible and determine its irreducible constituents. First, we change the basis to diagonalize the matrix of Frobenius. We see that

$$P_i\left(0\right)=\left\{\begin{array}{ll} R\left(\bar{\beta}_i,\bar{\gamma}_i\right), & \text{with } \{\bar{\beta}_i,\bar{\gamma}_i\}=\{1,p^{k_i}\} \text{ if } P_i \text{ has type 2 or 4,}\\ \operatorname{diag}\left(\bar{\alpha}_i,\bar{\delta}_i\right), & \text{with } \{\bar{\alpha}_i,\bar{\delta}_i\}=\{1,p^{k_i}\} \text{ if } P_i \text{ has type 1 or 3,}\end{array}\right.$$

where $R\left(\bar{\beta}_i,\bar{\gamma}_i\right)$ is the 2×2 matrix with $\bar{\beta}_i$ in the $(1,2)$ entry, $\bar{\gamma}_i$ in the $(2,1)$ entry, and zero on the diagonal. Let $Q_0=Id$,

$$Q_1=\left\{\begin{array}{l} Id \text{ if } P_1\in\{t_1,t_3\},\\ R \ \text{ if } P_1\in\{t_2,t_4\},\end{array}\right.$$

where $R:=R\left(1,1\right)$,

$$Q_i=\left\{\begin{array}{l} Id \text{ if } Q_{i-1}=Id \text{ and } P_i\in\{t_1,t_3\},\\ R \text{ if } Q_{i-1}=Id \text{ and } P_i\in\{t_2,t_4\},\\ R \text{ if } Q_{i-1}=R \text{ and } P_i\in\{t_1,t_3\},\\ Id \text{ if } Q_{i-1}=R \text{ and } P_i\in\{t_2,t_4\}\end{array}\right. \tag{6.2}$$

for $i=2,3,...,2f-1$. Let $Q=\left(Q_0,Q_1,...,Q_{2f-1}\right)$. By the definition of the matrices Q_i, the matrix $Q\cdot P(\vec{0})^{\otimes 2}\cdot\varphi\left(Q^{-1}\right)$ is diagonal. By induction, $Q_0=Id$ and

$$Q_i=\left\{\begin{array}{l} Id \text{ if an even number of coordinates}\\ \text{of } \left(P_1,P_2,...,P_i\right) \text{ is of even type,}\\ \\ R \text{ if an odd number of coordinates}\\ \text{of } \left(P_1,P_2,...,P_i\right) \text{ is of even type,}\end{array}\right. \tag{6.3}$$

for $i=1,2,...,2f-1$, where $P_{i+f}=P_i$ for $i=0,1,...,f-1$. We claim that for each $i=0,1,...,f-1$, $Q_i=Id$ if and only if $Q_{i+f}=R$. Indeed, for $i=0$, $Q_0=Id$. Since an odd number of coordinates of $(P_1,P_2,...,P_f)$ is of even type, $Q_f=R$. Let q_{ij}^r be the r-th coordinate of the (i,j)-entry $\vec{q}_{ij}$ of Q for each $i,j\in\{1,2\}$ and $r\in\{0,1,...,2f-1\}$. Assume that $i\in\{1,2,...,f-1\}$. From the definition of the matrices Q_i we see that

$$q_{11}^i=\left\{\begin{array}{l} 1 \text{ if an even number of coordinates}\\ \text{of } \left(P_1,P_2,...,P_i\right) \text{ is of even type,}\\ \\ 0 \text{ if an odd number of coordinates}\\ \text{of } \left(P_1,P_2,...,P_i\right) \text{ is of even type.}\end{array}\right. \tag{6.4}$$

For any $i = 0, 1, ..., f-1$ we have

$$q_{11}^{i+f} = \begin{cases} 1 \text{ if an even number of coordinates of} \\ (P_1, P_2, ..., P_f, ...P_{i+f}) \text{ is of even type,} \\ \\ 0 \text{ if an odd number of coordinates of} \\ (P_1, P_2, ..., P_f, ...P_{i+f}) \text{ is of even type.} \end{cases} \tag{6.5}$$

Since an odd number of coordinates of $(P_1, P_2, ..., P_f)$ is of even type and $P_i = P_{i+f}$ for all i, this is equivalent to

$$q_{11}^{i+f} = \begin{cases} 1 \text{ if an odd number of coordinates} \\ \text{of } (P_1, P_2, ..., P_i) \text{ is of even type,} \\ \\ 0 \text{ if an even number of coordinates} \\ \text{of } (P_1, P_2, ..., P_i) \text{ is of even type,} \end{cases} \tag{6.6}$$

which implies that $q_{11}^{i+f} = 1 - q_{11}^{i}$ for all $i = 0, 1, ..., f-1$. Similarly $q_{ij}^{r+f} = 1 - q_{ij}^{r}$ for all entries ij. Consider the ordered basis $\underline{\zeta} = (\zeta_1, \zeta_2)$ defined by $(\zeta_1, \zeta_2) := (\eta_1, \eta_2)\, Q^{-1}$. In the ordered basis $\underline{\zeta}$ the filtration is as in formula 5.10 with the vector $\vec{x}\eta_1 + \vec{y}\eta_2$ replaced by $\vec{x} \cdot (\vec{q}_{11} \cdot \zeta_1 + \vec{q}_{12} \cdot \zeta_2) + \vec{y} \cdot (\vec{q}_{12} \cdot \zeta_1 + \vec{q}_{22} \cdot \zeta_2)$. Let $\vec{z} = \vec{x} \cdot \vec{q}_{11} + \vec{y} \cdot \vec{q}_{12}$ and $\vec{w} = \vec{x} \cdot \vec{q}_{12} + \vec{y} \cdot \vec{q}_{22}$. From the definition of the matrices Q_i, the matrix of Frobenius in this new basis is the diagonal matrix

$$\operatorname{diag}\left(\vec{\lambda}, \vec{\mu}\right) := \left(Q_0 \cdot P_1 \cdot Q_1^{-1}, ..., Q_{f-1} \cdot P_f \cdot Q_f^{-1}, Q_f \cdot P_{f+1} \cdot Q_{f+1}^{-1}, ..., Q_{2f-1} \cdot P_0 \cdot Q_0^{-1}\right).$$

We prove that $\mathrm{Nm}_\varphi(\vec{\lambda}) = \mathrm{Nm}_\varphi(\vec{\mu}) = p^{\sum_{i=0}^{f-1} k_i} \cdot \vec{1}$. First we see that $\lambda_i \mu_i = p^{k_i}$ for all i. Since $Q_i = Id$ if and only if $Q_{i+f} = R$, a case by case analysis for the choices of Q_i and Q_{i+1}, bearing in mind that $P_{i+f} = P_i$, implies that $Q_i \cdot P_{i+1} \cdot Q_{i+1}^{-1} = \operatorname{diag}(\lambda_{i+1}, \mu_{i+1})$ if and only if $Q_{i+f} \cdot P_{i+f+1} \cdot Q_{i+f+1}^{-1} = \operatorname{diag}(\mu_{i+1}, \lambda_{i+1})$. Therefore,

$$\begin{aligned} & \prod_{i=0}^{2f-1} \left(Q_i \cdot P_{i+1} \cdot Q_{i+1}^{-1}\right) \\ = & \prod_{i=0}^{f-1} \left(Q_i \cdot P_{i+1} \cdot Q_{i+1}^{-1}\right) \cdot \prod_{i=0}^{f-1} \left(Q_{i+f} \cdot P_i \cdot Q_{i+f+1}^{-1}\right) \\ = & \prod_{i=0}^{f-1} \operatorname{diag}(\lambda_{i+1}, \mu_{i+1}) \cdot \prod_{i=0}^{f-1} \operatorname{diag}(\mu_{i+1}, \lambda_{i+1}) = p^{\sum_{i=0}^{f-1} k_i} \cdot Id. \end{aligned}$$

Next we notice that $\vec{y} = \vec{1} - \vec{x}$ and $\vec{q}_{12} = \vec{1} - \vec{q}_{11}$, so $\vec{z} = \vec{x} \cdot \vec{q}_{11} + \left(\vec{1} - \vec{x}\right) \cdot \left(\vec{1} - \vec{q}_{11}\right) = \vec{1} + 2 \cdot \vec{x} \cdot \vec{q}_{11} - \vec{q}_{11} - \vec{x}$. Since x_i and $q_{11}^i \in \{0, 1\}$ for all i, $z_i = 0$ if and only if $q_{11}^{i} = 1$ and $x_i = 0$, or $q_{11}^{i} = 0$ and $x_i = 1$. Recall from formula 5.11 that $x_i = 0$ if and only if $P_i \in \{t_3, t_4\}$ and $x_i = 1$ if and only if $P_i \in \{t_1, t_2\}$. This combined with the definition of the matrices Q_i gives

$$z_i = 0 \Leftrightarrow \begin{cases} i = 0 \text{ and } P_0 \in \{t_3, t_4\}, \text{ or} \\ \\ i \geq 1,\ P_i \in \{t_3, t_4\} \text{ and an even number of coordinates} \\ \text{of } (P_1, P_2, ..., P_i) \text{ is of even type, or} \\ \\ i \geq 1,\ P_i \in \{t_1, t_2\} \text{ and an odd number of coordinates} \\ \text{of } (P_1, P_2, ..., P_i) \text{ is of even type.} \end{cases} \tag{6.7}$$

Similarly,

$$z_i = 1 \Leftrightarrow \begin{cases} i = 0 \text{ and } P_0 \in \{t_1, t_2\}, \text{ or} \\ \\ i \geq 1,\ P_i \in \{t_1, t_2\} \text{ and an even number of coordinates} \\ \text{of } (P_1, P_2, ..., P_i) \text{ is of even type,} \\ \\ i \geq 1,\ P_i \in \{t_3, t_4\} \text{ and an odd number of coordinates} \\ \text{of } (P_1, P_2, ..., P_i) \text{ is of even type.} \end{cases} \tag{6.8}$$

We claim that $z_{i+f} = 1 - z_i$ for all $i = 0, 1, ..., f-1$. Indeed, $z_{i+f} = 1 + 2 \cdot x_{i+f} \cdot q_{11}^{i+f} - q_{11}^{i+f} - x_{i+f}$. Since $P_i = P_{i+f}$, we have $x_i = x_{i+f}$ for all i, and since $q_{11}^{i+f} = 1 - q_{11}^{f}$ we get $z_{i+f} = 1 - z_i$. Since $z_i \in \{0, 1\}$ for all i,

$$\sum_{\substack{i=0 \\ z_i=0}}^{2f-1} k_i = \sum_{\substack{i=0 \\ z_i=0}}^{f-1} k_i + \sum_{\substack{i=0 \\ z_{i+f}=0}}^{f-1} k_i = \sum_{i=0}^{f-1} k_i.$$

Since $\mathrm{v_p}\left(\mathrm{Nm}_{\varphi}\left(\vec{\mu}\right)\right) = \sum_{i=0}^{f-1} k_i = \sum_{\substack{i=0 \\ z_i=0}}^{2f-1} k_i$, Proposition 6.3[1] implies that the representation $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ is reducible. If $\mathbb{D}_2 := \left(E^{|\tau_{K_{2f}}|}\right)\zeta_2$, by [Dou10, proof of Prop. 4.3] (or by a direct computation),

$$\mathrm{Fil}^{\mathrm{j}}\mathbb{D}_2 = \begin{cases} \mathbb{D}_2 & \text{if } j \leq 0, \\ \left(E^{|\tau_{K_{2f}}|} f_{I_{i,\vec{z}}}\right)\zeta_2 & \text{if } 1 + w_{i-1} \leq j \leq w_i,\ i = 0, 1, ..., t-1, \\ 0 & \text{if } j \geq 1 + w_{t-1}, \end{cases} \tag{6.9}$$

where $I_{i,\vec{z}} = I_i \cap \{j \in \{0, 1, ..., 2f-1\} : z_j = 0\}$. Let $i \in \{0, 1, ..., 2f-1\}$.

[1] F-semisimplicity is not assumed here, but the part of Proposition 6.3 used still holds.

Arguing as in Lemma 6.10 we see that

$$e_i\mathrm{Fil}^{\mathrm{j}}\mathbb{D}_2 = \begin{cases} e_i E^{|\tau_{K_{2f}}|}\zeta_2 & \text{if } j \le 0, \\ e_i \left(\sum\limits_{\substack{r=0 \\ z_r=0}}^{2f-1} e_i \right) E^{|\tau_{K_{2f}}|}\zeta_2 & \text{if } 1 \le j \le k_i, \\ 0 & \text{if } j \ge 1+k_i. \end{cases}$$

Hence

$$e_i\mathrm{Fil}^{\mathrm{j}}\mathbb{D}_2 = \begin{cases} e_i E^{|\tau_{K_{2f}}|}\zeta_2 & \text{if } j \le 0, \\ 0 & \text{if } j \ge 1 \end{cases}$$

if $z_i = 1$ and

$$e_i\mathrm{Fil}^{\mathrm{j}}\mathbb{D}_2 = \begin{cases} e_i E^{|\tau_{K_{2f}}|}\zeta_2 & \text{if } j \le k_i, \\ 0 & \text{if } j \ge 1+k_i \end{cases}$$

if $z_i = 0$. The labeled Hodge-Tate weight of $\mathbb{D}_2$ with respect to the embedding τ_i of K_{2f} into E is 0 if $z_i = 1$ and $-k_i$ if $z_i = 0$. Next we prove that

$$z_i = \begin{cases} 0 \text{ if } \ell_i = 0, \\ 1 \text{ if } \ell_i = k_i > 0 \end{cases}$$

for $i = 0, 1, ..., f-1$, and

$$z_{i+f} = \begin{cases} 1 \text{ if } \ell_i = 0, \\ 0 \text{ if } \ell_i = k_i > 0. \end{cases}$$

Since $z_{i+f} = 1 - z_i$ for all $i = 0, 1, ..., f-1$, it suffices to prove the first formula. Suppose that $\ell_1 = 0$. Then $P_1 \in \{t_2, t_3\}$ and by formula 6.7, $z_1 = 0$. If $\ell_1 = k_1 > 0$, then $P_1 \in \{t_1, t_4\}$ and formula 6.7 implies that $z_1 = 1$. Let $i \in \{1, 2, ..., f-2\}$ and assume that $\ell_i = 0$. If an even number of coordinates of $(P_1, P_2, ..., P_{i-1})$ is of even type, then $P_i \in \{t_2, t_3\}$ and formula 6.7 implies $z_i = 0$. Arguing similarly we see that if $\ell_i = k_i > 0$, formula 6.8 implies $z_i = 1$. Finally, assume that $i = f$ and $\ell_f = 0$. If an even number of coordinates of $(P_1, P_2, ..., P_{f-1})$ is of even type, then $P_0 = P_f = t_4$ and formula 6.7 implies that $z_0 = z_f = 0$. We finish the proof by verifying similarly the remaining cases. By the formulas above, the labeled Hodge-Tate weight of $\mathbb{D}_2$ with respect to the embedding τ_i is

$$\begin{cases} -k_i \text{ if } \ell_i = 0, \\ 0 \quad \text{if } \ell_i = k_i > 0 \end{cases}$$

for $i = 0, 1, ..., f-1$ and

$$\begin{cases} -k_i \text{ if } \ell_i = k_i > 0, \\ 0 \quad \text{if } \ell_i = 0 \end{cases}$$

for $i = f, f+1, ..., 2f-1$. Therefore the labeled Hodge-Tate weight of $\mathbb{D}_2$ with respect to the embedding τ_i is

$$\begin{cases} -(k_i - \ell_i) & \text{if } i = 0, 1, ..., f-1 \\ -\ell_i & \text{if } i = f, f+1, ..., 2f-1. \end{cases}$$

Since $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$ for all $i = 0, 1, ..., f-1$, the labeled Hodge-Tate weights of $\mathbb{D}_2$ are $(-\ell_0, -\ell_1, ..., -\ell_{f-1}, -\ell_f, -\ell_{f+1}, ..., -\ell_{2f-1})$. Since $\mathrm{Nm}_{\varphi}(\vec{\mu}) = p^{\sum_{i=0}^{f-1} k_i} \cdot \vec{1}$, Proposition 3.5 implies that the crystalline character corresponding to $\mathbb{D}_2$ is $\chi_{e_0}^{\ell_1} \cdot \chi_{e_1}^{\ell_2} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}} \cdot \chi_{e_{2f-1}}^{\ell_0}$. Suppose that $V_{\vec{k}}^{\vec{i}}(\vec{0})$ is reducible. Then there exists some irreducible constituent of $V_{\vec{k}}^{\vec{i}}(\vec{0})$ whose restriction to $G_{K_{2f}}$ is $\chi_{e_0}^{\ell_1} \cdot \chi_{e_1}^{\ell_2} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}} \cdot \chi_{e_{2f-1}}^{\ell_0}$. Since the labeled weights of the latter character are $(-\ell_0, -\ell_1, ..., -\ell_{f-1}, -\ell_f, ..., -\ell_{2f-1})$, Corollary 2.7 implies that $\ell_i = \ell_{i+f}$ for all $i = 0, 1, ..., f-1$. Since $\{\ell_i, \ell_{i+f}\} = \{0, k_i\}$ for $i = 0, 1, ..., f-1$, and since some labeled weight is strictly positive this is absurd. Hence $V_{\vec{k}}^{\vec{i}}(\vec{0})$ is irreducible and its restriction to $G_{K_{2f}}$ contains $\chi_{e_0}^{\ell_1} \cdot \chi_{e_1}^{\ell_2} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}} \cdot \chi_{e_{2f-1}}^{\ell_0}$ as an irreducible constituent. By Frobenius reciprocity,

$$V_{\vec{k}}^{\vec{i}}(\vec{0}) = \mathrm{Ind}_{K_{2f}}^{K_f} \left(\chi_{e_0}^{\ell_1} \cdot \chi_{e_1}^{\ell_2} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}} \cdot \chi_{e_{2f-1}}^{\ell_0} \right).$$

This finishes the proof of part (i). Part (ii) follows from Theorem 4.7 and parts (iii) and (4) follow from Corollary 6.9. For part (iv), notice that any irreducible induced member of $V_{\vec{k}}^{\vec{i}}(\vec{a})$ has the form $\eta_c \cdot \mathrm{Ind}_{K_{2f}}^{K_f} \left(\chi_{e_0}^{\ell_1'} \cdot \chi_{e_1}^{\ell_2'} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}'} \cdot \chi_{e_{2f-1}}^{\ell_0'} \right)$ for some unramified character η_c and some nonnegative integers with $\{\ell_i', \ell_{i+f}'\} = \{0, k_i\}$ for all i (see Proposition 3.11). All the members of $V_{\vec{k}}^{\vec{i}}(\vec{a})$ have determinant $(-1)^t p^{\sum_{i=0}^{f-1} k_i}$, where t is the number of even coordinates of $\vec{i}$. This equals the determinant of $\mathrm{Ind}_{K_{2f}}^{K_f} \left(\chi_{e_0}^{\ell_1'} \cdot \chi_{e_1}^{\ell_2'} \cdot \cdots \cdot \chi_{e_{2f-2}}^{\ell_{2f-1}'} \cdot \chi_{e_{2f-1}}^{\ell_0'} \right)$ and forces the unramified character η_c to be trivial. Hence the only irreducible induced member of our family is $V_{\vec{k}}^{\vec{i}}(\vec{0})$. ∎

Remark 6.13. *Let R be as in the proof of Proposition 6.12. If $\mathcal{A}$ is a set of 2×2 matrices, let $R\mathcal{A} := \{R \cdot A : A \in \mathcal{A}\}$ and $\mathcal{A}R := \{A \cdot R : A \in \mathcal{A}\}$. We write $\{t_i, t_j\}$ for a set which contains matrices of type t_i and t_j. Then $R\{t_1, t_2\} = \{t_1, t_2\}$, $R\{t_3, t_4\} = \{t_3, t_4\}$, $\{t_1, t_2\}R = \{t_3, t_4\}$ and $\{t_3, t_4\}R = \{t_1, t_2\}$. In the definition of the matrices P_i we may always assume that $P_i \in \{t_1, t_2\}$ for all $i = 1, 2, ...f-1$. Indeed, let $Q_0 = R$, and for $i = 1, 2, ..., f-1$ let*

$$Q_i = \begin{cases} Id \text{ if } P_i \in \{t_1, t_2\}, \\ R \;\text{ if } P_i \in \{t_3, t_4\}. \end{cases}$$

After changing the basis by the matrix $Q = (Q_0, Q_1, ..., Q_{f-1})$ we have $P_i \in \{t_1, t_2\}$ for all $i = 1, 2, ...f-1$. By the definition preceding Proposition 6.12, the type of the matrix $P_0 \in \{t_1, t_2, t_3, t_4\}$ is uniquely determined by $(P_1, P_2, ..., P_{f-1})$.

Theorem 6.14. *Theorem 1.5 holds.*

Proof. Follows from Proposition 6.12 and Remark 6.13. □

EXAMPLE 6.15. *Let $f = 2$ and $k_i > 0$ for $i = 0, 1$. Up to twist by some unramified character, there exist two distinct isomorphism classes of irreducible two-dimensional crystalline E-representations of G_{K_2} with labeled Hodge-Tate weights $(\{0, -k_0\}, \{0, -k_1\})$ induced from crystalline characters of G_{K_4}.*
(i) If $\ell_0 = k_0$ and $\ell_1 = k_1$, then from the definition of the matrices Π_i preceding Proposition 6.12 and Remark 6.13, $(\Pi_1, \Pi_0) = (t_1, t_2)$. Let $P_i = \Pi_i \bmod \pi$. The polynomials z_i in the definition of the matrices Π_i are such that $z_i \equiv p^m \bmod \pi$, where $m := \lfloor \frac{\max\{k_0,k_1\}-1}{p-1} \rfloor$, unless $k_0 = k_1 = p$ in which case we define $m = 0$. For any $\vec{a} = (a_0, a_1) \in \mathfrak{m}_E^2$ we consider the family of crystalline representations $V_{\vec{k},\vec{a}}^{(1,2)}$ constructed in §5.2. The corresponding family of filtered φ-modules is $\left(\mathbb{D}_{\vec{k},\vec{a}}^{(1,2)}, \varphi\right)$, with $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2) P^{(1,2)}(\vec{a})$, where

$$P^{(1,2)}(\vec{a}) = \begin{pmatrix} (p^{k_1}, a_0 p^m) & (0,1) \\ (a_1 p^m, p^{k_0}) & (1,0) \end{pmatrix},$$

and the filtrations are

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}_{\vec{k},\vec{a}}^{(1,2)}) = \begin{cases} E^2\eta_1 \bigoplus E^2\eta_2 & \text{if } \ j \leq 0, \\ E^2(\vec{x}\cdot\eta_1 + \vec{y}\cdot\eta_2) & \text{if } \ 1 \leq j \leq w_0, \\ E^1 f_{I_1}(\vec{x}\cdot\eta_1 + \vec{y}\cdot\eta_2) & \text{if } \ 1 + w_0 \leq j \leq w_1, \\ 0 & \text{if } \ j \geq 1 + w_1, \end{cases} \tag{6.10}$$

with $w_0 = \min\{k_0, k_1\}$ and $w_1 = \max\{k_0, k_1\}$,

$$f_{I_1} = \begin{cases} (0,1) & \text{if } \ k_0 < k_1, \\ (1,0) & \text{if } \ k_1 < k_0, \\ (0,0) & \text{if } \ k_0 = k_1, \end{cases}$$

and $(\vec{x}, \vec{y}) = ((1,1), (0,0))$. We have

$$V_{\vec{k},\vec{0}}^{(1,2)} \simeq \mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_0}^{k_1} \cdot \chi_{e_3}^{k_0}\right),$$

and for any $\vec{a} \in \mathfrak{m}_E^2$,

$$\left(\left(\overline{V}_{\vec{k},\vec{a}}^{(1,2)}\right)_{|I_{K_2}}\right)^{s.s.} \simeq \omega_{4,\bar{\tau}_0}^{-(k_0+pk_1)} \bigoplus \omega_{4,\bar{\tau}_0}^{-(k_0+pk_1)p^2}.$$

Let $\alpha_i = a_i p^m$ and $A = \alpha_1 + p^{k_1}\alpha_0$. Assume that $A^2 \neq -4p^{k_0+k_1}$ and let $\varepsilon_0 \neq \varepsilon_1$ be the distinct roots of the characteristic polynomial $X^2 - A\cdot X + p^{k_0+k_1}$. Arguing as in the proof of Proposition 2.2 in [Dou10], we get the following "standard parametrization" for the family $V_{\vec{k},\vec{a}}^{(1,2)}$,

$$\varphi(\eta_1) = (1, \varepsilon_0)\,\eta_1, \ \ \varphi(\eta_2) = \left(\lambda, \frac{\varepsilon_1}{\lambda}\right)\eta_2,$$

where

$$\lambda = \lambda(\alpha_0) = \frac{\varepsilon_1}{\varepsilon_0} \cdot \frac{\left(\varepsilon_1 - A + p^{k_1}\alpha_0\right)}{\left(\varepsilon_0 - A + p^{k_1}\alpha_0\right)}$$

(notice that $\varepsilon_i \neq A - \alpha_0 p^{k_1}$), and filtrations are as in Formula 6.10 with $\vec{x} = \vec{y} = \vec{1}$.
(ii) If $\ell_0 = \ell_1 = 0$. Again, taking into account Remark 6.13, we may only consider the case $(\Pi_1, \Pi_0) = (t_2, t_3)$. For each $\vec{a} \in \mathfrak{m}_E^2$ consider the family $V_{\vec{k},\vec{a}}^{(2,3)}$ of two-dimensional crystalline E-representations of G_{K_2} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$, $i = 0, 1$. We have

$$V_{\vec{k},\vec{0}}^{(2,3)} \simeq \mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_2}^{k_1} \cdot \chi_{e_1}^{k_0}\right) \simeq \mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_0}^{k_1} \cdot \chi_{e_3}^{k_0}\right).$$

For any $\vec{a} \in \mathfrak{m}_E^2$,

$$\left(\left(\overline{V}_{\vec{k},\vec{a}}^{(2,3)}\right)_{|I_{K_2}}\right)^{s.s.} \simeq \omega_{4,\tau_0}^{-(k_0+pk_1)} \bigoplus \omega_{4,\tau_0}^{-(k_0+pk_1)p^2}.$$

Notice that the family $\left\{V_{\vec{k},\vec{a}}^{(1,2)},\ \vec{a} \in \mathfrak{m}_E^2\right\}$ of case (i) coincides with the family $\left\{V_{\vec{k},\vec{a}}^{(2,3)},\ \vec{a} \in \mathfrak{m}_E^2\right\}$, as the second family is obtained from the first one by changing the basis by the matrix $Q = (R, R)$.
(iii) Let $f = 2$, $\ell_0 = 0$ and $\ell_1 = k_1 > 0$. Then $(\Pi_1, \Pi_0) = (t_1, t_4)$. For each $\vec{a} \in \mathfrak{m}_E^2$ consider the family $V_{\vec{k},\vec{a}}^{(1,4)}$ of two-dimensional crystalline E-representations of G_{K_2} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$, $i = 0, 1$. Then

$$V_{\vec{k},\vec{0}}^{(1,4)} \simeq \mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_0}^{k_1} \cdot \chi_{e_1}^{k_0}\right),$$

and for any $\vec{a} \in \mathfrak{m}_E^2$,

$$\left(\left(\overline{V}_{\vec{k},\vec{a}}^{(1,4)}\right)_{|I_{K_2}}\right)^{s.s.} \simeq \omega_{4,\bar{\tau}_0}^{-\left(pk_1+p^2k_0\right)} \bigoplus \omega_{4,\bar{\tau}_0}^{-\left(pk_1+p^2k_0\right)p^2}.$$

Let $\alpha_i = a_i p^m$ and $A = \alpha_0 + p^{k_0}\alpha_1$. Assume that $A^2 \neq -4p^{k_0+k_1}$ and let $\varepsilon_0 \neq \varepsilon_1$ be the distinct roots of the characteristic polynomial $X^2 - A \cdot X + p^{k_0+k_1}$. Arguing as in the proof of Proposition 2.2 in [Dou10], we get the following "standard parametrization" for the family $V_{\vec{k},\vec{a}}^{(1,4)}$,

$$\varphi(\eta_1) = (1, \varepsilon_0)\,\eta_1,\ \varphi(\eta_2) = \left(\lambda, \frac{\varepsilon_1}{\lambda}\right)\eta_2,$$

where

$$\lambda = \lambda(\alpha_1) = \left(\frac{\varepsilon_1}{\varepsilon_0}\right)^2 \cdot \frac{\left(A - p^{k_0}\alpha_1 - \varepsilon_0\right)}{\left(A - p^{k_0}\alpha_1 - \varepsilon_1\right)}$$

(notice that $\varepsilon_i \neq A - \alpha_1 p^{k_0}$), and filtrations as in Formula 6.10 with $\vec{x} = \vec{y} = \vec{1}$.
(iv) If $f = 2$ $\ell_0 = k_0 > 0$ and $\ell_1 = 0$. Then $(\Pi_1, \Pi_0) = (t_2, t_1)$ and this gives the family obtained in case (iii).

Example 6.16. *If $f=2$, $k_0>0$ and $k_1=0$. Then up to unramified twist, $\mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_3}^{k_0}\right)$ is a unique isomorphism class of two-dimensional crystalline irreducible E-representations of G_{K_2} with labeled weights $(\{0,-k_0\},\{0,0\})$ induced from G_{K_4}. We have*

$$V_{\vec{k},\vec{0}}^{(2,3)} \simeq \mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_3}^{k_0}\right) \simeq \mathrm{Ind}_{K_4}^{K_2}\left(\chi_{e_1}^{k_0}\right),$$

and for any $\vec{a}\in\mathfrak{m}_E^2$,

$$\left(\left(\overline{V}_{\vec{k},\vec{a}}^{(2,3)}\right)_{|I_{K_2}}\right)^{s.s.} \simeq \omega_{4,\bar{\tau}_0}^{-k_0} \bigoplus \omega_{4,\bar{\tau}_0}^{-p^2k_0}.$$

Example 6.17. *Let $f=3$, $k_i>0$ for all $i=0,1,2$. Up to twist by some unramified character, there exist 4 distinct isomorphism classes of irreducible two-dimensional crystalline E-representations of G_{K_3} with labeled Hodge-Tate weights $(\{0,-k_0\},\{0,-k_1\},\{0,-k_2\})$ induced from G_{K_6}. One of those classes is represented by $\mathrm{Ind}_{K_6}^{K_3}\left(\chi_{e_0}^{k_1}\cdot\chi_{e_1}^{k_2}\cdot\chi_{e_2}^{k_0}\right)$. For the families containing it we have $\ell_i=k_i>0$ for all $i=0,1,2$. Since $k_0>0$, $\Pi_0=t_2$ if $\Pi_2=t_4$ and $\Pi_0=t_1$ if $\Pi_2=t_1$. Hence $(\Pi_1,\Pi_2,\Pi_0)\in\{(t_4,t_4,t_2),(t_4,t_1,t_1),(t_1,t_2,t_1),(t_1,t_3,t_2)\}$. By Remark 6.13 we may only consider the case $(\Pi_1,\Pi_2,\Pi_0)=(t_1,t_2,t_1)$. For any $\vec{a}\in\mathfrak{m}_E^3$, consider the the families $V_{\vec{k},\vec{a}}^{(1,2,1)}$ of two-dimensional crystalline E-representations of G_{K_3} with labeled Hodge-Tate weights $\{0,-k_i\}_{\tau_i}$, $i=0,1,2$. We have*

$$V_{\vec{k},\vec{0}}^{(1,2,1)} \simeq \mathrm{Ind}_{K_6}^{K_3}\left(\chi_{e_0}^{k_1}\cdot\chi_{e_1}^{k_2}\cdot\chi_{e_2}^{k_0}\right),$$

and for any $\vec{a}\in\mathfrak{m}_E^3$,

$$\left(\left(\overline{V}_{\vec{k},\vec{a}}^{(1,2,1)}\right)_{|I_{K_3}}\right)^{s.s.} \simeq \omega_{6,\bar{\tau}_0}^{-\left(k_0+pk_1+p^2k_2\right)} \bigoplus \omega_{6,\bar{\tau}_0}^{-\left(k_0+pk_1+p^2k_2\right)p^3}.$$

6.3 Proof of theorem 1.7

Let $V_{\vec{\ell},\vec{\ell}'}(\eta)=\eta\cdot\chi_{e_0}^{\ell_1}\cdot\chi_{e_1}^{\ell_2}\cdot\dots\cdot\chi_{e_{f-1}}^{\ell_0}\bigoplus\chi_{e_0}^{\ell_1'}\cdot\chi_{e_1}^{\ell_2'}\cdot\dots\cdot\chi_{e_{f-1}}^{\ell_0'}$ with $\{\ell_i,\ell_i'\}=\{0,k_i\}$ for all i, where $\eta=\eta_c$ is the unramified character of G_{K_f} which maps the geometric Frobenius Frob_{K_f} of G_{K_f} to $c\in\mathcal{O}_E^{\times}$. As usual, we assume that at least one k_i is strictly positive. We choose f-tuples of matrices $(\Pi_1,\Pi_2,...,\Pi_f)$ (with $\Pi_f=\Pi_0$) as follows:
(1) If $\ell_1=0$, $\Pi_1\in\{t_2,t_3\}$;
(2) If $\ell_1=k_1>0$, $\Pi_1\in\{t_1,t_4\}$.
For $i=2,3,...,f-1$, we choose the type of the matrix Π_i as follows:
(1) If $\ell_i=0$, then:

- If an even number of coordinates of $(\Pi_1,\Pi_2,...,\Pi_{i-1})$ is of even type, $\Pi_i\in\{t_2,t_3\}$;
- If an odd number of coordinates of $(\Pi_1,\Pi_2,...,\Pi_{i-1})$ is of even type, $\Pi_i\in\{t_1,t_4\}$.

(2) If $\ell_i = k_i > 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{i-1})$ is of even type, $\Pi_i \in \{t_1, t_4\}$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{i-1})$ is of even type, $\Pi_i \in \{t_2, t_3\}$.

Finally, we choose the type of the matrix Π_0 as follows:
(1) If $\ell_0 = 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_3$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_4$.

(2) If $\ell_0 = k_i > 0$, then:

- If an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_1$;
- If an odd number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_{f-1})$ is of even type, $\Pi_0 = t_2$.

Notice that the type of Π_0 has been chosen so that an even number of coordinates of $(\Pi_1, \Pi_2, ..., \Pi_f)$ is of even type. We choose the units c_i appearing in the entries of the matrices Π_i in Definition 5.4 so that $c_i = 1$ for all $i = 1, 2, ..., f-1$, and $c_0 = c$. Let $\vec{i}$ be the type-vector attached to $(\Pi_1, \Pi_2, ..., \Pi_f)$. We exclude those vectors $\vec{i}$ for which $(\Pi_1, \Pi_2, ..., \Pi_f) \in C_1 \cup C_2$, which is to exclude the cases where $\vec{\ell} = \vec{0}$ or $\vec{\ell'} = \vec{0}$. For any $\vec{a} \in \mathfrak{m}_E^f$ we consider the families of crystalline E-representations $V_{\vec{k}}^{\vec{i}}(\vec{a})$ of G_{K_f} with labeled Hodge-Tate weights $\{0, -k_i\}_{\tau_i}$ constructed in §5.2.

Proposition 6.18. *(i) For any type vector $\vec{i}$ chosen as above there exists some unramified character μ such that $\mu \otimes V_{\vec{k}}^{\vec{i}}(\vec{0}) \simeq V_{\vec{\ell}, \vec{\ell'}}(\eta)$;*

(ii) For any $\vec{a} \in \mathfrak{m}_E^f$, $\overline{V}_{\vec{k}}^{\vec{i}}(\vec{a}) \simeq \overline{V}_{\vec{k}}^{\vec{i}}(\vec{0})$ and

$$\left(\overline{V}_{\vec{k}}^{\vec{i}}(\vec{a})\right)_{|I_{K_f}} \simeq \left(\overline{V}_{\vec{\ell}, \vec{\ell'}}(\eta)\right)_{|I_{K_f}} \simeq \omega_{f, \bar{\tau}_0}^{\alpha} \oplus \omega_{f, \bar{\tau}_0}^{\alpha'},$$

where $\alpha = -\sum_{i=i}^{f-1} \ell_i p^i$ and $\alpha' = -\sum_{i=0}^{f-1} \ell'_i p^i$.

Proof. For simplicity assume that $\eta = 1$. The general case follows by choosing the unit c_0 in the definition of Π_0 appropriately. We restrict $V_{\vec{k}}^{\vec{i}}(\vec{0})$ to $G_{K_{2f}}$. By the construction of the representation $V_{\vec{k}}^{\vec{i}}(\vec{0})$ in §5.1, there exists some G_{K_f}-stable lattice $\left(\mathrm{T}_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{G_{K_f}}$ inside $V_{\vec{k}}^{\vec{i}}(\vec{0})$ whose Wach module has φ-action defined by $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2) \cdot \Pi(\vec{0})$. By Proposition 2.6, the Wach module of the $G_{K_{2f}}$-stable lattice $\left(\mathrm{T}_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ inside $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ is defined by $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2) \cdot \Pi(0)^{\otimes 2}$, therefore the filtered φ-module corresponding to $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ has Frobenius endomorphism $(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2) \cdot P(0)^{\otimes 2}$. The restricted representation $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ has labeled weights $(\{0, -k_i\})_{\tau_i}$, $i = 0, 1, ..., 2f-1$, with $k_{i+f} = k_i$ for $i = 0, 1, ..., f-1$, and filtration as in formula 5.10 for some vectors $\vec{x}, \vec{y}$, with the sets I_j being defined with respect to the $2f$ weights above. We prove that $\left(V_{\vec{k}}^{\vec{i}}(\vec{0})\right)_{|G_{K_{2f}}}$ is reducible and determine its irreducible constituents. First we change the basis to diagonalize the matrix of Frobenius. We define matrices Q_i as in the proof of Proposition 6.12, and we let $Q = (Q_0, Q_1, ..., Q_{2f-1})$. By the definition of the matrices Q_i, the matrix $Q \cdot P(0)^{\otimes 2} \cdot \varphi\left(Q^{-1}\right)$ is diagonal. By the proof of Proposition 6.12, $Q_0 = Id$ and for $i = 1, 2, ..., 2f-1$, Q_i is as in formula 6.3. We claim that for each $i = 0, 1, ..., f-1$, $Q_i = Q_{i+f}$. Indeed, from the definition of the matrices Q_i we see that q_{11}^{i} and q_{11}^{i+f} are as in formulas 6.4 and 6.5 respectively in the proof of Proposition 6.12. Since an even number of coordinates of $(P_1, P_2, ..., P_f)$ are of even type, $q_{11}^{i+f} = q_{11}^{i}$. Similarly, $q_{ij}^{r+f} = q_{ij}^{r}$ for any entry (i, j). Consider the ordered basis $\underline{\zeta} = (\zeta_1, \zeta_2)$ defined by $(\zeta_1, \zeta_2) := (\eta_1, \eta_2) \cdot Q^{-1}$. Let $\vec{q}_{ij}$ be th (i, j)-entry of Q. In the new basis $\underline{\zeta}$ the filtration is as in formula 5.10 with the vector $\vec{x}\eta_1 + \vec{y}\eta_2$ replaced by $\vec{x} \cdot (\vec{q}_{11} \cdot \zeta_1 + \vec{q}_{12} \cdot \zeta_2) + \vec{y} \cdot (\vec{q}_{12} \cdot \zeta_1 + \vec{q}_{22} \cdot \zeta_2)$. Let $\vec{z} = \vec{x} \cdot \vec{q}_{11} + \vec{y} \cdot \vec{q}_{12}$ and $\vec{w} = \vec{x} \cdot \vec{q}_{12} + \vec{y} \cdot \vec{q}_{22}$. The matrix of Frobenius in this new basis is the diagonal matrix diag $\left(\vec{\lambda}, \vec{\mu}\right)$. Arguing as in Proposition 6.12, and taking into account that $q_{ij}^{r+f} = q_{ij}^{r}$ for all $r = 0, 1, ..., f-1$ and all entries (i, j) we see that $z_{r+f} = z_r$ for all r. From the proof of the same proposition, $z_i = 0$ if and only if $q_{11}^{i} = 1$ and $x_i = 0$ or $q_{11}^{i} = 0$ and $x_i = 1$. Formula 5.11 implies that $x_i = 0$ if and only if $P_i \in \{t_4, t_3\}$ and $x_i = 1$ if and only if $P_i \in \{t_2, t_1\}$. Since $z_i = z_{i+f}$ and $k_i = k_{i+f}$ for all $i = 0, 1, ..., f-1$,

$$\sum_{\substack{i=0 \\ z_i=0}}^{2f-1} k_i = 2\sum_{\substack{i=0 \\ z_i=0}}^{f-1} k_i = 2\sum_{\substack{i=0 \\ Q_i=R \\ P_i=t_1}}^{f-1} k_i + 2\sum_{\substack{i=0 \\ Q_i=R \\ P_i=t_2}}^{f-1} k_i + 2\sum_{\substack{i=0 \\ Q_i=Id \\ P_i=t_3}}^{f-1} k_i + 2\sum_{\substack{i=0 \\ Q_i=Id \\ P_i=t_4}}^{f-1} k_i.$$

We now show that the $(2,2)$ entry of $\prod_{i=0}^{2f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)$ is the p^n, where

$$n = 2\sum_{\substack{i=0\\ Q_i=R\\ P_i=t_1}}^{f-1} k_i + 2\sum_{\substack{i=0\\ Q_i=R\\ P_i=t_2}}^{f-1} k_i + 2\sum_{\substack{i=0\\ Q_i=Id\\ P_i=t_3}}^{f-1} k_i + 2\sum_{\substack{i=0\\ Q_i=Id\\ P_i=t_4}}^{f-1} k_i. \tag{6.11}$$

Since the matrices $Q_iP_{i+1}Q_{i+1}^{-1}$ are diagonal, and since $Q_{i+f} = Q_i$ and $P_{i+f} = P_i$ for all i,

$$\begin{aligned}\prod_{i=0}^{2f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right) = &\prod_{\substack{i=0\\ Q_i=Id\\ P_{i+1}=t_4}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot \prod_{\substack{i=0\\ Q_i=Id\\ P_{i+1}=t_3}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot \\ \prod_{\substack{i=0\\ Q_i=Id\\ P_{i+1}=t_1}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot &\prod_{\substack{i=0\\ Q_i=Id\\ P_{i+1}=t_2}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot \prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_4}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot \\ \prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_3}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot &\prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_1}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 \cdot \prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_2}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)^2 .\end{aligned}$$

We notice that when $Q_i = Id$ and $P_{i+1} = t_4$, then by formula 6.2, $Q_{i+1} = R$ and $Q_iP_{i+1}Q_{i+1}^{-1} = \operatorname{diag}\left(p^{k_{i+1}}, 1\right)$. Therefore the product $\prod_{\substack{i=0\\ Q_i=Id\\ P_{i+1}=t_4}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)$ has no contribution to the $(2,2)$ entry of $\prod_{i=0}^{2f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)$. Similarly, the products

$$\prod_{\substack{i=0\\ Q_i=Id\\ P_{i+1}=t_1}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right), \prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_3}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right) \text{ and } \prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_2}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)$$

have no contribution to the $(2,2)$ entry of $\prod_{i=0}^{2f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)$. We now compute the product $\prod_{\substack{i=0\\ Q_i=R\\ P_{i+1}=t_1}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)$. Formula 6.2 implies that if $Q_i = R$ and $P_{i+1} = t_1$ then $Q_{i+1} = R$, therefore $Q_iP_{i+1}Q_{i+1}^{-1} = \operatorname{diag}\left(1, p^{k_{i+1}}\right)$. Again, by formula 6.2, $Q_i = R$ and $P_{i+1} = t_1$ is equivalent to $Q_{i+1} = R$ and $P_{i+1} = t_1$. Hence

$$\prod_{\substack{i=0\\Q_i=R\\P_{i+1}=t_1}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)=\prod_{\substack{i=0\\Q_{i+1}=R\\P_{i+1}=t_1}}^{f-1}\left(Q_iP_{i+1}Q_{i+1}^{-1}\right)=\prod_{\substack{i=0\\Q_i=R\\P_i=t_1}}^{f-1}\operatorname{diag}\left(1,p^{k_{i+1}}\right)$$

which contributes the fourth summand of the right hand side of equation 6.11. The claim made before formula 6.11 follows arguing similarly for the remaining cases. Hence $\mathrm{v_p}\left(\mathrm{Nm}_\varphi\left(\vec{\mu}\right)\right)=\sum\limits_{\substack{i=0\\z_i=0}}^{2f-1}k_i$. Proposition 6.3 implies that $\left(V_{\vec{k},\vec{0}}^{\vec{i}}\right)_{|G_{K_{2f}}}$ is reducible and $(\mathbb{D}_2,\varphi)$ is a weakly admissible submodule, where $\mathbb{D}_2=\left(E^{2f}\right)\cdot\zeta_2$. By [Dou10, proof of Prop. 4.3] (or by a direct computation),

$$\mathrm{Fil^j}\mathbb{D}_2=\begin{cases}\mathbb{D}_2 & \text{if}\quad j\leq 0,\\ \left(E^{|\tau_{K_{2f}}|}\right)f_{I_{i,\vec{z}}}\zeta_2 & \text{if}\ \ 1+w_{i-1}\leq j\leq w_i \text{ for all } i=0,1,...,t-1,\\ 0 & \text{if}\ \ j\geq 1+w_{t-1},\end{cases}\tag{6.12}$$

where $I_{i,\vec{z}}=I_i\cap\{j\in\{0,1,...,2f-1\}:z_j=0\}$. As in the proof of Proposition 6.12, the labeled weight for the embedding τ_i is 0 if $z_i=1$ and $-k_i$ if $z_i=0$. Next, we prove that for $i=0,1,...,f-1$,

$$z_i=z_{i+f}=\begin{cases}0 \text{ if } \ell_i=0,\\ 1 \text{ if } \ell_i=k_i>0.\end{cases}\tag{6.13}$$

This is proved exactly as in Proposition 6.12, taking into account that an even number of the coordinates of $(P_1,P_2,...,P_f)$ is of even type. We have $z_i=0$ for all i if and only if $\ell_i=0$ for all i if and only if $(\Pi_1,\Pi_2,...,\Pi_f)\in C_1$ and $z_i=1$ for all i if and only if $\ell_i=k_i>0$ for all i if and only if $(\Pi_1,\Pi_2,...,\Pi_f)\in C_2$, cases excluded. Therefore neither of the summands of $V_{\vec{k}}^{\vec{i}}(\vec{0})$ is unramified. By the discussion above the labeled weights of $\mathbb{D}_2$ are $\left(-\ell'_0,-\ell'_1,...,-\ell'_{f-1},-\ell'_0,-\ell'_1,...,-\ell'_{f-1}\right)$. By formula 6.13, $\mathrm{v_p}\left(\mathrm{Nm}_\varphi\left(\vec{\mu}\right)\right)=\sum\limits_{\substack{i=0\\z_i=0}}^{2f-1}k_i=\sum\limits_{i=0}^{2f-1}\ell'_i$. By Proposition 3.5 and Lemma 3.7, the corresponding crystalline character is $\psi=\chi_{e_0}^{\ell'_1}\cdot\chi_{e_1}^{\ell'_2}\cdot\dots\cdot\chi_{e_{f-2}}^{\ell'_{f-1}}\cdot\chi_{e_{f-1}}^{\ell'_0}\cdot\chi_{e_0}^{\ell'_1}\cdot\chi_{e_1}^{\ell'_2}\cdot\dots\cdot\chi_{e_{f-2}}^{\ell'_{f-1}}\cdot\chi_{e_{f-1}}^{\ell'_0}$. If $V_{\vec{k}}^{\vec{i}}(\vec{0})$ is irreducible, then by Frobenius reciprocity $V_{\vec{k}}^{\vec{i}}(\vec{0})=\mathrm{Ind}_{K_{2f}}^{K_f}\left(\psi\right)$, which is absurd by Corollary 3.10. Hence $V_{\vec{k}}^{\vec{i}}(\vec{0})$ is reducible and contains an irreducible constituent which restricts to ψ. By Lemma 3.7(iv) the only choices are $\eta_{\pm 1}\cdot\chi_{e_0}^{\ell_1}\cdot\chi_{e_1}^{\ell_2}\cdot\dots\cdot\chi_{e_{f-2}}^{\ell_{f-1}}\cdot\chi_{e_{f-1}}^{\ell_0}$, and we are done after twisting by $\eta_{\mp 1}$. The rest of the proposition follows as in the proof of Proposition 6.12. □

THEOREM 6.19. *Theorem 1.7 holds.*

Proof. Follows from Proposition 6.18, taking into account Remark 6.13. □

Example 6.20. *Let $f = 2$, $\ell_0 = 0$ and $\ell_1 = k_1$. Let $(\Pi_1, \Pi_0) = (t_1, t_3)$ with $c_0 = c_1 = 1$. After possibly twisting by $\eta_{\pm 1}$ we have $V_{\vec{k}}^{(1,3)}(\vec{0}) \simeq \chi_{e_0}^{k_1} \oplus \chi_{e_1}^{k_0}$.*

In the next proposition we study closer the F-semisimple members of this family assuming that $c = 1$.

Proposition 6.21. *Assume that $V_{\vec{k}}^{(1,3)}(\vec{\alpha})$ is F-semisimple.*

(i) $V_{\vec{k}}^{(1,3)}(\vec{\alpha})$ is irreducible if and only if $\alpha_0\alpha_1 \neq 0$, and is non-induced for all but finitely many such $\vec{\alpha}$;

(ii) $V_{\vec{k}}^{(1,3)}(\vec{\alpha})$ is non-split reducible if and only if precisely one of the coordinates α_i of $\vec{\alpha}$ is zero;

(iii) The families $\left\{V_{\vec{k}}^{(1,3)}((\alpha_0, 0)),\ \alpha_0 \in p^m\mathfrak{m}_E \setminus \{0\}\right\}$ and $\left\{V_{\vec{k}}^{(1,3)}((0, \alpha_1)),\ \alpha_1 \in p^m\mathfrak{m}_E \setminus \{0\}\right\}$ are disjoint;

(iv) $V_{\vec{k}}^{(1,3)}(\vec{0})$ is split-reducible.

Proof. The weakly admissible filtered φ-module corresponding to $V_{\vec{k}}^{(1,3)}(\vec{\alpha})$ has Frobenius endomorphism

$$(\varphi(\eta_1), \varphi(\eta_2)) = (\eta_1, \eta_2)\begin{pmatrix} (p^{k_1}, 1) & (0, \alpha_0) \\ (\alpha_1, 0) & (1, p^{k_0}) \end{pmatrix}$$

and filtration

$$\mathrm{Fil}^{\mathrm{j}}(\mathbb{D}) = \begin{cases} (E\times E)\eta_1 \bigoplus (E\times E)\eta_2 & \text{if } j \leq 0, \\ (E\times E) f_{I_0}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } 1 \leq j \leq w_0, \\ (E\times E) f_{I_1}(\vec{x}\eta_1 + \vec{y}\eta_2) & \text{if } 1 + w_0 \leq j \leq w_1, \\ 0 & \text{if } j \geq 1 + w_1, \end{cases} \tag{6.14}$$

with $\vec{x} = (-\alpha_0, 1)$ and $\vec{y} = (1, -\alpha_1)$. We diagonalize the matrix of Frobenius arguing as in the proof of Proposition 2.2 in [Dou10]. The characteristic polynomial is $X^2 - \left(p^{k_0} + p^{k_1} + \alpha_0\alpha_1\right)X + p^{k_0+k_1}$, and we assume that $\left(p^{k_0} + p^{k_1} + \alpha_0\alpha_1\right)^2 \neq 4p^{k_0+k_1}$ so that its roots ε_0 and ε_1 are distinct. We have the following cases.

Case (1). $\alpha_0\alpha_1 \neq 0$. We change the basis to $\underline{\xi} = (\xi_1, \xi_2)$, where

$$\xi_1 = \left(\left(\varepsilon_0 - p^{k_1} - \alpha_0\alpha_1\right)\alpha_1,\ \frac{\alpha_0(\varepsilon_0-\varepsilon_1)\left(\varepsilon_0 - p^{k_0}\right)\left(\varepsilon_0 - p^{k_0} - \alpha_0\alpha_1\right)\left(\varepsilon_1 - p^{k_1} - \alpha_0\alpha_1\right)}{\left(2\varepsilon_0\varepsilon_1 - p^{k_0}\varepsilon_1 - p^{k_1}\varepsilon_0 - \alpha_0\alpha_1\varepsilon_1\right)\left(\varepsilon_1 - p^{k_0} - \alpha_0\alpha_1\right)}\right)\eta_1$$

$$+ \left(\left(\varepsilon_0 - p^{k_1} - \alpha_0\alpha_1\right)\alpha_1,\ \frac{\alpha_0(\varepsilon_0-\varepsilon_1)\left(\varepsilon_1 - p^{k_0}\right)\left(\varepsilon_0 - p^{k_0} - \alpha_0\alpha_1\right)\left(\varepsilon_1 - p^{k_1} - \alpha_0\alpha_1\right)}{\left(2\varepsilon_0\varepsilon_1 - p^{k_0}\varepsilon_1 - p^{k_1}\varepsilon_0 - \alpha_0\alpha_1\varepsilon_1\right)\left(\varepsilon_1 - p^{k_0} - \alpha_0\alpha_1\right)}\right)\eta_2$$

and

$$\xi_2 = \left(\left(\varepsilon_1 - p^{k_1} - \alpha_0\alpha_1\right)\left(\varepsilon_0 - p^{k_1}\right),\ \frac{\alpha_0^2(\varepsilon_0-\varepsilon_1)\left(\varepsilon_1-p^{k_1}-\alpha_0\alpha_1\right)\left(\varepsilon_1-p^{k_0}-\alpha_0\alpha_1\right)}{\left(2\varepsilon_0\varepsilon_1-p^{k_0}\varepsilon_1-p^{k_1}\varepsilon_0-\alpha_0\alpha_1\varepsilon_1\right)\left(\varepsilon_1-p^{k_0}-\alpha_0\alpha_1\right)} \right)\eta_1$$

$$+ \left(\left(\varepsilon_1 - p^{k_1} - \alpha_0\alpha_1\right)\left(\varepsilon_1 - p^{k_1}\right),\ \frac{\alpha_0^2(\varepsilon_0-\varepsilon_1)\left(\varepsilon_1-p^{k_1}-\alpha_0\alpha_1\right)\left(\varepsilon_1-p^{k_0}-\alpha_0\alpha_1\right)}{\left(2\varepsilon_0\varepsilon_1-p^{k_0}\varepsilon_1-p^{k_1}\varepsilon_0-\alpha_0\alpha_1\varepsilon_1\right)\left(\varepsilon_1-p^{k_0}-\alpha_0\alpha_1\right)} \right)\eta_2$$

In the ordered basis $\underline{\xi}$ we have $\varphi(\xi_1) = (1,\ \varepsilon_0)\,\xi_1$ and $\varphi(\xi_2) = \left(\lambda,\ \frac{\varepsilon_1}{\lambda}\right)\xi_2$, where

$$\lambda = -\frac{\left(\varepsilon_0 - p^{k_1} - \alpha_0\alpha_1\right)}{\left(\varepsilon_1 - p^{k_1} - \alpha_0\alpha_1\right)} \cdot \frac{\left(\varepsilon_1 - p^{k_0} - \alpha_0\alpha_1\right)}{\left(\varepsilon_0 - p^{k_0} - \alpha_0\alpha_1\right)} \cdot \frac{\left(2\varepsilon_0\varepsilon_1 - p^{k_0}\varepsilon_1 - p^{k_1}\varepsilon_0 - \alpha_0\alpha_1\varepsilon_1\right)}{\left(2\varepsilon_0\varepsilon_1 - p^{k_0}\varepsilon_0 - p^{k_1}\varepsilon_1 - \alpha_0\alpha_1\varepsilon_0\right)},$$

and the filtration is as in formula 6.14, with $\vec{x}\eta_1 + \vec{y}\eta_2$ replaced by $\xi_1 + \xi_2$. By Proposition 6.3, the representation $V_{\vec{k}}^{(1,3)}(\vec{\alpha})$ is irreducible. Arguing as in the proof of Proposition 6.12(iv) we see that the representations $V_{\vec{k}}^{(1,3)}(\vec{\alpha})$ are non-induced with the possibility of at most finitely many exceptions.

Case (2). $\alpha_0 = 0$, $\alpha_1 \neq 0$. We argue as above and see that in the ordered basis $\underline{\xi} = (\xi_1, \xi_2)$, where

$$\xi_1 = \eta_2 \text{ and } \xi_2 = \left(1,\ \frac{p^{k_0} - p^{k_1}}{\alpha_1 p^{k_1}}\right)\eta_1 - \left(\frac{\alpha_1}{p^{k_0} - p^{k_1}},\ p^{k_0 - k_1}\right)\eta_2$$

we have $\varphi(\xi_1) = \left(1,\ p^{k_0}\right)\xi_1$ and $\varphi(\xi_2) = \left(\lambda(\alpha_1),\ \frac{p^{k_1}}{\lambda(\alpha_1)}\right)\xi_2$, with $\lambda(\alpha_1) = \alpha_1^{-1}\left(p^{k_0} - p^{k_1}\right)$. The filtration in this basis is given by formula 6.14, with $\vec{x}\eta_1 + \vec{y}\eta_2$ replaced by $\xi_1 + (0,1)\,\xi_2$. By Proposition 6.3 the representation $V_{\vec{k}}^{(1,3)}((0,\alpha_1))$ is reducible and non-split.

Case (3). $\alpha_1 = 0, \alpha_0 \neq 0$. In the ordered basis $\underline{\xi} = (\xi_1, \xi_2)$, where

$$\xi_1 = \eta_2 - \left(\frac{p^{k_1}\alpha_0}{p^{k_1} - p^{k_0}},\ \frac{\alpha_0}{p^{k_1} - p^{k_0}}\right)\eta_1 \text{ and } \xi_2 = \left(\frac{\alpha_0 p^{k_0}}{p^{k_1} - p^{k_0}},\ 1\right)\eta_1,$$

we have $\varphi(\xi_1) = \left(1,\ p^{k_0}\right)\xi_1$ and $\varphi(\xi_2) = \left(\lambda(\alpha_0),\ \frac{p^{k_1}}{\lambda(\alpha_0)}\right)\xi_2$, with $\lambda(\alpha_0) = \alpha_0^{-1}\left(p^{k_1} - p^{k_0}\right)p^{k_1 - k_0}$. The filtration in the basis ξ is given by formula 6.14, with $\vec{x}\eta_1 + \vec{y}\eta_2$ replaced by $(1,0)\,\xi_1 + \xi_2$. By Proposition 6.3, $V_{\vec{k}}^{(1,3)}((\alpha_0,0))$ is reducible, non-split. By [Dou10, Proposition 7.1] it follows that there are no isomorphisms between members of the families $\left\{V_{\vec{k}}^{(1,3)}((\alpha_0,0)),\ \alpha_0 \in p^m\mathfrak{m}_E \setminus \{0\}\right\}$ and $\left\{V_{\vec{k}}^{(1,3)}((0,\alpha_1)),\ \alpha_1 \in p^m\mathfrak{m}_E \setminus \{0\}\right\}$.

Case (4). $\alpha_0 = \alpha_1 = 0$. Then $\varphi(\eta_1) = \left(p^{k_1}, 1\right)\eta_1$ and $\varphi(\eta_2) = \left(1, p^{k_0}\right)\eta_2$, while the filtration is as in formula 6.14,with $\vec{x} = (0,1)$ and $\vec{y} = (1,0)$. Since $J_{\vec{x}} \cap J_{\vec{y}} = \varnothing$, Proposition 6.3 implies that $V_{\vec{k}}^{(1,3)}(\vec{0})$ is split-reducible. □

Proposition 6.22. *Let $0 < \mathrm{v_p}(\varepsilon_i) < k_0 + k_1$ with $\varepsilon_0 \neq \varepsilon_1$ such that $\varepsilon_0\varepsilon_1 = p^{k_0+k_1}$ and assume that $0 \leq k_i \leq p-1$. Define the families of filtered φ-modules $\mathbb{D}(\lambda)$ with*

$$\varphi(\eta_1) = (1, \varepsilon_0)\,\eta_1,\ \varphi(\eta_2) = \left(\lambda, \frac{\varepsilon_1}{\lambda}\right)\eta_2,$$

and filtrations as in formula 6.10 with $\vec{x} = \vec{y} = \vec{1}$. These filtered modules are weakly admissible, irreducible, sharing the same characteristic polynomial and filtration. Let $V(\lambda)$ be the corresponding to $\mathbb{D}(\lambda)$ crystalline representations of $G_{\mathbb{Q}_{p^2}}$.

(i) If $\lambda = \frac{\varepsilon_1}{\varepsilon_0}\left(\frac{p^{k_1}\alpha-\varepsilon_0}{p^{k_1}\alpha-\varepsilon_1}\right)$, where $\alpha \in m_E$, then $\left(\overline{V(\lambda)}_{|I_{\mathbb{Q}_{p^2}}}\right)^{ss} = \omega_{4,\bar{\tau}_0}^{-(k_0+pk_1)} \bigoplus \omega_{4,\bar{\tau}_0}^{-(k_0+pk_1)p^2}$ and $\overline{V(\lambda)}$ is irreducible;

(ii) If $\lambda = \left(\frac{\varepsilon_1}{\varepsilon_0}\right)^2\left(\frac{p^{k_1}\alpha-\varepsilon_1}{p^{k_1}\alpha-\varepsilon_0}\right)$, where $\alpha \in m_E$, then $\left(\overline{V(\lambda)}_{|I_{\mathbb{Q}_{p^2}}}\right)^{ss} = \omega_{4,\bar{\tau}_0}^{-(pk_1+p^2k_0)} \bigoplus \omega_{4,\bar{\tau}_0}^{-(pk_1+p^2k_0)p^2}$ and $\overline{V(\lambda)}$ is irreducible;

(iii) If $\lambda = 1$, then $\overline{V(\lambda)}$ is reducible and $\overline{V(\lambda)}_{|I_{\mathbb{Q}_{p^2}}} = \omega_{2,\bar{\tau}_0}^{-k_1} \bigoplus \omega_{2,\bar{\tau}_0}^{-pk_0}$.

Proof. The common characteristic polynomial is $X^2 - (\varepsilon_0 + \varepsilon_1)X + p^{k_0+k_1}$. Parts (i) and (ii) follow from Examples 6.15 (i) and (iii) using the "standard parametrization" for the families $V_{\vec{k},\vec{a}}^{(1,2)}$ and $V_{\vec{k},\vec{a}}^{(1,4)}$, and taking into account that $m = 0$ and Proposition 6.8. Part (iii) follows from Proposition 6.21(i) and a little computation to prove that if $p^{k_0} + p^{k_1} + \alpha_0\alpha_1 = \varepsilon_0 + \varepsilon_1$ and $\varepsilon_0\varepsilon_1 = p^{k_0+k_1}$, then $\lambda = 1$. □

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Fuss-Catalan Numbers in Noncommutative Probability

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Abstract. We prove that if $p, r \in \mathbb{R}$, $p \geq 1$ and $0 \leq r \leq p$ then the Fuss-Catalan sequence $\binom{mp+r}{m}\frac{r}{mp+r}$ is positive definite. We study the family of the corresponding probability measures $\mu(p, r)$ on $\mathbb{R}$ from the point of view of noncommutative probability. For example, we prove that if $0 \leq 2r \leq p$ and $r + 1 \leq p$ then $\mu(p, r)$ is $\boxplus$-infinitely divisible. As a by-product, we show that the sequence $\frac{m^m}{m!}$ is positive definite and the corresponding probability measure is $\boxtimes$-infinitely divisible.

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1. Introduction

For natural numbers m, p, r let $A_m(p, r)$ denote the number of all sequences $(a_1, a_2, \ldots, a_{mp+r})$ such that: (1) $a_i \in \{1, 1-p\}$, (2) $a_1 + a_2 + \ldots + a_s > 0$ for all s such that $1 \leq s \leq mp + r$ and (3) $a_1 + a_2 + \ldots + a_{mp+r} = r$. It turns out that this is given by the two-parameter Fuss-Catalan numbers (2.1) (see [5, 13]). Note that the right hand side of (2.1) allows us to define $A_m(p, r)$ for all *real* parameters p and r. In particular, the *Catalan numbers* $A_m(2, 1)$ are known as moments of the Marchenko–Pastur distribution:

$$d\widetilde{\pi}(x) = \frac{1}{2\pi}\sqrt{\frac{4-x}{x}}dx \qquad \text{on } [0, 4], \tag{1.1}$$

which in the free probability theory plays the role of the Poisson measure. In this paper we are going to study the question for which parameters $p, r \in \mathbb{R}$

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the sequence $\{A_m(p,r)\}_{m=0}^{\infty}$ is positive definite, i.e. is the moment sequence of some probability measure (which we will denote $\mu(p,r)$). Recently T. Banica, S. T. Belinschi, M. Capitaine and B. Collins [1] showed that if $p>1$ then $\{A_m(p,1)\}_{m=0}^{\infty}$ is the moment sequence of a probability measure which can be expressed as the multiplicative free power $\widetilde{\pi}^{\boxtimes p-1}$.
We are going to prove that if $p,r\in\mathbb{R}$, $p\geq 1$ and $0\leq r\leq p$ then $\{A_m(p,r)\}_{m=0}^{\infty}$ is the moment sequence of a unique probability measure $\mu(p,r)$ which has compact support contained in $[0,\infty)$. Moreover, if $0\leq 2r\leq p$ and $r+1\leq p$ then $\mu(p,r)$ is infinitely divisible with respect to the free convolution $\boxplus$. In some particular cases we are able to determine the multiplicative free convolution, the boolean power and the monotonic convolution of the measures $\mu(p,r)$. We will also prove that if $0\leq r\leq p-1$ then the sequence $\left\{\binom{mp+r}{m}\right\}_{m=0}^{\infty}$ is positive definite and the corresponding probability measure can be expressed as $\mu(p-r,1)^{\uplus p}\rhd\mu(p,r)$, where $\uplus$ and $\rhd$ denote the boolean and the monotonic convolution, respectively.
The paper is organized as follows. In Section 2 we prove three combinatorial identities. Then we use them to derive some formulas for the generating functions. In Section 4 we regard the numbers $A_m(p,r)$ as moments of a *probability quasi-measure* $\mu(p,r)$ (by this we mean a linear functional $\mu:\mathbb{R}[x]\to\mathbb{R}$ satisfying $\mu(1)=1$). On the class of probability quasi-measures one can introduce the free, boolean and monotonic convolutions in combinatorial way. The class of compactly supported probability measures on $\mathbb{R}$, regarded as a subclass of the former, is closed under these operations. We prove some formulas involving the probability quasi measures $\mu(p,r)$, for example we find the free R- and S-transforms (4.8), (4.11), the boolean powers $\mu(p,1)^{\uplus t}$ (4.18) and, in special cases, the multiplicative free (4.12), (4.13), (4.14) and the monotonic convolution (4.20) of the measures $\mu(p,r)$.
In Section 5 we prove that if $p\geq 1$ and $0\leq r\leq p$ then $\mu(p,r)$ is a measure (we conjecture that this condition is also necessary for $p,r>0$). The proof involves the multiplicative free convolution $\boxtimes$. Moreover, we show that if $0\leq 2r\leq p$ and $r+1\leq p$ then $\mu(p,r)$ is $\boxplus$-infinitely divisible.
In the final part we extend our results to the dilations of the measures $\mu(p,r)$, with parameter $h>0$. Taking the limit with $h\to 0$ we prove in particular that the sequence $\left\{\frac{m^m}{m!}\right\}_{m=0}^{\infty}$ is positive definite and the corresponding probability measure ν_0 is $\boxtimes$-infinitely divisible.

2. Some combinatorial identities

We will work with the two-parameter Fuss-Catalan numbers (see [5, 13]) defined by: $A_0(p,r):=1$ and

$$A_m(p,r):=\frac{r}{m!}\prod_{i=1}^{m-1}(mp+r-i) \tag{2.1}$$

for $m \geq 1$, where p, r are real parameters. Note that (2.1) can be written as $\binom{mp+r}{m}\frac{r}{mp+r}$, unless $mp + r = 0$. One can check that for $m \geq 0$

$$A_m(p, r) = A_m(p, r-1) + A_{m-1}(p, p+r-1), \tag{2.2}$$

under convention that $A_{-1}(p, r) := 0$, and

$$A_m(p, p) = A_{m+1}(p, 1). \tag{2.3}$$

It is also known (see [13]) that

$$\sum_{k=0}^{m} A_k(p, r)A_{m-k}(p, s) = A_m(p, r+s). \tag{2.4}$$

Now we are going to prove three identities, valid for $c, d, p, r, t \in \mathbb{R}$, which will be needed later on.

Proposition 2.1.

$$\sum_{k=0}^{m} A_k(p-r, c)A_{m-k}(p, kr+d) = A_m(p, c+d). \tag{2.5}$$

Proof. It is easy to check that the formula is true for $m = 0$ and $m = 1$. Denoting the left hand side by $S_m(p, r, c, d)$ we have from (2.2):

$$\begin{aligned}
S_m(p, r, c, d) &= \sum_{k=0}^{m} A_k(p-r, c)A_{m-k}(p, kr+d) \\
&= \sum_{k=0}^{m} \left[A_k(p-r, c-1) + A_{k-1}(p-r, p-r+c-1)\right] A_{m-k}(p, kr+d) \\
&= \sum_{k=0}^{m} A_k(p-r, c-1)A_{m-k}(p, kr+d) \\
&\qquad + \sum_{k=1}^{m} A_{k-1}(p-r, p-r+c-1)A_{m-k}(p, kr+d) \\
&= S_m(p, r, c-1, d) + \sum_{k=0}^{m-1} A_k(p-r, p-r+c-1)A_{m-1-k}(p, kr+r+d) \\
&= S_m(p, r, c-1, d) + S_{m-1}(p, r, p-r+c-1, r+d),
\end{aligned}$$

so that we have

$$S_m(p, r, c, d) = S_m(p, r, c-1, d) + S_{m-1}(p, r, p-r+c-1, r+d).$$

Fix m and assume that (2.5) holds for $m-1$. Now we prove that for m it holds for every natural c. Indeed, it holds for $c = 0$ and if it does for $c-1$ then, by assumption and by (2.2):

$$\begin{aligned}
S_m(p, r, c, d) &= S_m(p, r, c-1, d) + S_{m-1}(p, r, p-r+c-1, r+d) \\
&= A_m(p, c+d-1) + A_{m-1}(p, p+c+d-1) = A_m(p, c+d),
\end{aligned}$$

which proves that the statement is true for c. Therefore it holds for all natural c. Now we note that both sides of (2.5) are polynomials on c of order m, therefore the formula holds for all $c \in \mathbb{R}$, which completes the inductive step. □

Proposition 2.2.

$$(1-t)\sum_{l=0}^{m} A_l\big(p,1\big)\sum_{j=0}^{m-l} A_{m-l-j}\big(p, j(p-1)+r\big)t^j + t\sum_{j=0}^{m} A_{m-j}\big(p, j(p-1)+r\big)t^j = A_m\big(p, r+1\big). \tag{2.6}$$

Proof. Using first (2.4) and then (2.2) we obtain:

$$\begin{aligned}
&t\sum_{j=0}^{m} A_{m-j}(p, j(p-1)+r)t^j \\
&\qquad + (1-t)\sum_{l=0}^{m} A_l\big(p,1\big)\sum_{j=0}^{m-l} A_{m-l-j}\big(p, j(p-1)+r\big)t^j \\
&= t\sum_{j=0}^{m} A_{m-j}(p, j(p-1)+r)t^j \\
&\qquad + (1-t)\sum_{j=0}^{m}\sum_{l=0}^{m-j} A_l(p,1)A_{m-j-l}(p, j(p-1)+r)t^j \\
&= t\sum_{j=0}^{m} A_{m-j}(p, j(p-1)+r)t^j \\
&\qquad + (1-t)\sum_{j=0}^{m} A_{m-j}(p, j(p-1)+r+1)t^j \\
&= \sum_{j=0}^{m} A_{m-j}(p, j(p-1)+r+1)t^j - \sum_{j=0}^{m-1} A_{m-j-1}(p, j(p-1)+r+p)t^{j+1} \\
&= A_m(p, r+1).
\end{aligned}$$

□

Proposition 2.3.

$$\sum_{k=0}^{m} A_{m-k}(p, k(p-1)+r)p^k = \binom{mp+r}{m}. \tag{2.7}$$

Proof. Denoting the left hand side by $T_m(p,r)$ we use (2.2) and get

$$\begin{aligned} T_m(p,r) &= \\ &= \sum_{k=0}^{m} A_{m-k}(p, k(p-1)+r)p^k \\ &= \sum_{k=0}^{m} \left[A_{m-k}(p, k(p-1)+r-1) + A_{m-1-k}(p, k(p-1)+p+r-1)\right] p^k \\ &= T_m(p, r-1) + T_{m-1}(p, p+r-1). \end{aligned}$$

Now we proceed as in the proof of (2.5), using the binomial identity

$$\binom{mp+r}{m} = \binom{mp+r-1}{m} + \binom{mp+r-1}{m-1}. \qquad \square$$

3. Generating functions

In this part we are going to study the generating functions

$$\mathcal{B}_p(z) := \sum_{m=0}^{\infty} A_m(p,1) z^m, \tag{3.1}$$

which are convergent in some neighborhood of 0 (to observe this one can use the inequality

$$|A_m(p,r)| \le |r| \left[m(|p|+1)+|r|\right]^{m-1}/m!$$

and apply the Cauchy's radical test). From (2.4) and (2.3) we have

$$\mathcal{B}_p(z)^r = \sum_{m=0}^{\infty} A_m(p,r) z^m \tag{3.2}$$

and

$$\mathcal{B}_p(z) = 1 + z\mathcal{B}_p(z)^p. \tag{3.3}$$

Indeed, denoting the right hand side of (3.2) by $\mathcal{A}_{p,r}(z)$ we have $\mathcal{A}_{p,1}(z) = \mathcal{B}_p(z)$ and, by (2.4), $\mathcal{A}_{p,r}(z) \cdot \mathcal{A}_{p,s}(z) = \mathcal{A}_{p,r+s}(z)$, which implies that $\mathcal{A}_{p,r}(z) = \mathcal{B}_p(z)^r$. Taking $r = p$ and applying (2.3) we get (3.3).
Now we are going to interpret formulas (2.5), (2.6), (2.7) in terms of these generating functions.

Proposition 3.1. *For any real parameters p, r we have*

$$\mathcal{B}_{p-r}\left(z\mathcal{B}_p(z)^r\right) = \mathcal{B}_p(z). \tag{3.4}$$

Proof. First we note that if $A(z) = \sum_{m=0}^{\infty} a_m z^m$, $B(z) = \sum_{n=1}^{\infty} b_n z^n$ then

$$A(B(z)) = a_0 + \sum_{m=1}^{\infty} z^m \sum_{k=1}^{m} a_k \sum_{\substack{i_1, i_2, \ldots, i_k \ge 1 \\ i_1+i_2+\ldots+i_k = m}} b_{i_1} b_{i_2} \ldots b_{i_k}. \tag{3.5}$$

Putting $b_i := A_{i-1}(p,r)$ for fixed k, m we have:

$$\sum_{\substack{i_1,i_2,\ldots,i_k\geq 1\\ i_1+i_2+\ldots+i_k=m}} b_{i_1}b_{i_2}\ldots b_{i_k} = \sum_{\substack{j_1,j_2,\ldots,j_k\geq 0\\ j_1+j_2+\ldots+j_k=m-k}} A_{j_1}(p,r)A_{j_2}(p,r)\ldots A_{j_k}(p,r)$$
$$= A_{m-k}(p,kr),$$

the coefficient of $\mathcal{B}_p(z)^{kr}$ at z^{m-k}. Now we put $a_k := A_k(p-r,1)$ and applying (2.5), with $c=1$, $d=0$, we get

$$\sum_{k=1}^{m} a_k \sum_{\substack{i_1,i_2,\ldots,i_k\geq 1\\ i_1+i_2+\ldots+i_k=m}} b_{i_1}b_{i_2}\ldots b_{i_k} \tag{3.6}$$
$$= \sum_{k=0}^{m} A_k(p-r,1)A_{m-k}(p,kr) = A_m(p,1),$$

as $A_m(p,0)=0$ for $m\geq 1$, which completes the proof. □

Note that in the proof we applied (2.5) only with $c=1$ and $d=0$.
For $p,r,t\in\mathbb{R}$ we denote

$$\mathcal{D}_{p,r,t}(z) := \frac{\mathcal{B}_p(z)^{1+r}}{(1-t)\mathcal{B}_p(z)+t}. \tag{3.7}$$

Proposition 3.2. *For $p,r,t\in\mathbb{R}$ we have*

$$\mathcal{D}_{p,r,t}(z) = \sum_{m=0}^{\infty} z^m \sum_{k=0}^{m} A_{m-k}(p,k(p-1)+r)t^k, \tag{3.8}$$

in particular:

$$\mathcal{D}_{p,r,p}(z) = \sum_{m=0}^{\infty}\binom{mp+r}{m}z^m. \tag{3.9}$$

Moreover

$$\mathcal{D}_{p-r,s,t}\left(z\mathcal{B}_p(z)^r\right)\mathcal{B}_p(z)^r = \mathcal{D}_{p,r+s,t}(z). \tag{3.10}$$

Proof. Using (2.6) we can verify that

$$\big[(1-t)\mathcal{B}_p(z)+t\big]\cdot\left[\sum_{m=0}^{\infty} z^m\sum_{k=0}^{m}A_{m-k}(p,k(p-1)+r)t^k\right] = \mathcal{B}_p(z)^{1+r}$$

which proves (3.8). Formulas (3.9) and (3.10) are consequences of (2.7) and (3.4). □

Proposition 3.3. *In some neighborhood of* 0 *we have*

$$\mathcal{B}_p\big(z(1+z)^{-p}\big) = 1+z, \tag{3.11}$$

and more generally, for $r\neq 0$ we have

$$\mathcal{B}_p\left(\big((1+z)^{\frac{1}{r}}-1\big)(1+z)^{\frac{-p}{r}}\right)^r = 1+z. \tag{3.12}$$

Proof. Since we have $\mathcal{B}_p(0) = 1$ and $\mathcal{B}'_p(0) = 1$, there is a function f_p defined on a neighborhood of 0 such that $f_p(0) = 0$ and $\mathcal{B}(f_p(z)) = 1+z$. Substituting $z \mapsto f_p(z)$ in (3.3) we obtain $f_p(z) = z(1+z)^{-p}$. Now we put $z \mapsto (1+w)^{1/r} - 1$ to (3.11) and taking the r-th power we obtain (3.12). □

Remark. Note that (3.11) leads to an analytic proof of (3.4). Namely, substituting in (3.4) $z \mapsto z(1+z)^{-p}$ we get

$$\begin{aligned}\mathcal{B}_{p-r}\left(z(1+z)^{-p}\mathcal{B}_p\left(z(1+z)^{-p}\right)^r\right) &= \mathcal{B}_{p-r}\left(z(1+z)^{-p}(1+z)^r\right)\\ &= 1+z = \mathcal{B}_p\left(z(1+z)^{-p}\right).\end{aligned}$$

Finally we note a symmetry possessed by our generating functions.

Proposition 3.4. *For $p, r, t \in \mathbb{R}$ we have*

$$\mathcal{B}_p(-z)^r = \mathcal{B}_{1-p}(z)^{-r}, \tag{3.13}$$

$$\mathcal{D}_{p,r,t}(-z) = \mathcal{D}_{1-p,-1-r,1-t}(z). \tag{3.14}$$

Proof. One can check that $(-1)^m A_m(p,r) = A_m(1-p,-r)$, which proves (3.13), and by the definition (3.7), (3.13) implies (3.14). □

4. Relations with noncommutative probability

By a *probability quasi-measure* we will mean a linear functional μ on the set $\mathbb{R}[x]$ of polynomials with real coefficients, satisfying $\mu(1) = 1$. In the case when μ is given by $\mu(P) = \int P(t)\, d\widetilde{\mu}(t)$ for some probability measure $\widetilde{\mu}$ on $\mathbb{R}$ we will identify μ with $\widetilde{\mu}$ and say that μ is *proper* or is just a *probability measure*. A probability quasi-measure μ is uniquely determined by its *moment sequence* $\{\mu(x^m)\}_{m=0}^{\infty}$. It is proper if and only if its moment sequence is *positive definite*, i.e. if

$$\sum_{i,j=0}^{\infty} \mu(x^{i+j})\alpha_i\alpha_j \geq 0$$

holds for every sequence $\{\alpha_i\}_{i=0}^{\infty}$ of real numbers, with only finitely many nonzero entries. All probability measures encountered in this paper are compactly supported and therefore uniquely determined by their moment sequences. For a probability quasi-measure μ we define its *moment generating function*, which is the (at least formal) power series

$$M_\mu(z) := \sum_{m=0}^{\infty} \mu(x^m) z^m$$

and its *reflection* $\widehat{\mu}$ by $\widehat{\mu}(x^m) := (-1)^m \mu(x^m)$ or, equivalently, $M_{\widehat{\mu}}(z) := M_\mu(-z)$. If μ is a probability measure then so is $\widehat{\mu}$ and then we have $\widehat{\mu}(X) = \mu(-X)$ for every Borel subset of $\mathbb{R}$.

For $p, r, t \in \mathbb{R}$ we define probability quasi-measures $\mu(p,r)$ and $\nu(p,r,t)$ by

$$\mu(p,r)(x^m) := A_m(p,r), \tag{4.1}$$

$$\nu(p,r,t)(x^m) := \sum_{k=0}^{m} A_{m-k}(p, k(p-1)+r)t^k, \tag{4.2}$$

in particular, by (2.7),

$$\nu(p,r,p)(x^m) = \binom{mp+r}{m}. \tag{4.3}$$

For example, $\mu(1,1) = \nu(1,0,1) = \delta_1$ and for every $p \in \mathbb{R}$ we have $\mu(p,0) = \nu(0,0,0) = \delta_0$. Note that $\nu(p,r,0) = \mu(p,r)$ so that the class of probability quasi-measures $\mu(p,r)$ is contained in that of $\nu(p,r,t)$, we will be interested however mainly in the former.
First we note that Proposition 3.4 leads to

Proposition 4.1.

$$\widehat{\mu(p,r)} = \mu(1-p,-r), \tag{4.4}$$

$$\widehat{\nu(p,r,t)} = \nu(1-p,-1-r,1-t). \qquad \square \tag{4.5}$$

There are several convolutions of probability quasi-measures, apart from the classical one: $(\mu * \nu)(x^n) := \sum_{k=0}^{n} \binom{n}{k} \mu(x^k)\nu(x^{n-k})$, which are related to various notions of independence (namely, the free, boolean and the monotonic independence) in noncommutative probability.

1. *Free convolution* (see [2, 15, 11]) is defined in the following way. For a probability quasi-measure μ we define its *free R-transform* (or the *additive free transform*) $R_\mu(z)$ by the formula:

$$M_\mu(z) = R_\mu(zM_\mu(z)) + 1. \tag{4.6}$$

The *free cumulants* $r_m(\mu)$ are defined as the coefficients of the Taylor expansion $R_\mu(z) = \sum_{k=1}^{\infty} r_k(\mu) z^k$ (combinatorial relation between moments and free cumulants is described in [11] and [4]). Then the free convolution $\mu \boxplus \nu$ can be defined as the unique probability quasi-measure which satisfies

$$R_{\mu\boxplus\nu}(z) = R_\mu(z) + R_\nu(z). \tag{4.7}$$

We also define *free power* $\mu^{\boxplus t}$, $t > 0$, by $R_{\mu^{\boxplus t}}(z) := tR_\mu(z)$.
As a consequence of (4.6) and (3.4) we obtain:

Proposition 4.2. *For the free additive transform of* $\mu(p,r)$ *we have*

$$R_{\mu(p,r)}(z) = \mathcal{B}_{p-r}(z)^r - 1 \tag{4.8}$$

so that for the free cumulants we have $r_m(\mu(p,r)) = A_m(p-r,r)$, $m \geq 1$. $\square$

The *free S-transform* (or the *free multiplicative transform*) of a quasi-measure μ, with $\mu(x^1) \neq 0$, is defined by the relation

$$R_\mu(zS_\mu(z)) = z \quad \text{or, equivalently,} \quad M_\mu\big(z(1+z)^{-1}S_\mu(z)\big) = 1 + z. \tag{4.9}$$

Then the *multiplicative free convolution* $\mu_1 \boxtimes \mu_2$ and the *multiplicative free power* $\mu^{\boxtimes t}$, $t > 0$, are defined by

$$S_{\mu_1 \boxtimes \mu_2}(z) := S_{\mu_1}(z) S_{\mu_2}(z) \quad \text{and} \quad S_{\mu^{\boxtimes t}}(z) := S_\mu(z)^t. \tag{4.10}$$

Proposition 4.3. *For $r \neq 0$ the S-transform of the measure $\mu(p,r)$ is equal to*

$$S_{\mu(p,r)}(z) = \frac{(1+z)^{\frac{1}{r}} - 1}{z} (1+z)^{\frac{r-p}{r}}. \tag{4.11}$$

Consequently

$$\mu(1+p_1, 1) \boxtimes \mu(1+p_2, 1) = \mu(1+p_1+p_2, 1), \tag{4.12}$$

and more generally

$$\mu(p_1, r) \boxtimes \mu(1+p_2, 1) = \mu(p_1 + r p_2, r). \tag{4.13}$$

We have also

$$\mu(1+p, 1)^{\boxtimes t} = \mu(1+tp, 1). \tag{4.14}$$

Proof. Formula (4.11) is a consequence of (3.12). In particular

$$S_{\mu(1+p,1)}(z) = (1+z)^{-p} \tag{4.15}$$

which leads to (4.12), (4.13) and (4.14). □

2. The *boolean convolution* $\mu_1 \uplus \mu_2$ and the boolean power $\mu^{\uplus t}$, $t > 0$, (see [14, 3]) can be defined by putting

$$\frac{1}{M_{\mu_1 \uplus \mu_2}(z)} = \frac{1}{M_{\mu_1}(z)} + \frac{1}{M_{\mu_2}(z)} - 1, \tag{4.16}$$

$$M_{\mu^{\uplus t}}(z) = \frac{M_\mu(z)}{(1-t) M_\mu(z) + t}. \tag{4.17}$$

Comparing this with definition (3.7) we get

Proposition 4.4. *For $p, t \in \mathbb{R}$ we have*

$$\mu(p,1)^{\uplus t} = \nu(p, 0, t). \quad \square \tag{4.18}$$

3. *Monotonic convolution* (see [10]) is an associative, noncommuting operation $\triangleright$ which is defined by: $\mu_1 \triangleright \mu_2 = \mu$ iff

$$M_\mu(z) = M_{\mu_1}\big(z M_{\mu_2}(z)\big) \cdot M_{\mu_2}(z). \tag{4.19}$$

Then (3.4) and (3.10) yield

Proposition 4.5. *For any parameters $a, b, r, t \in \mathbb{R}$ we have*

$$\mu(a,b) \triangleright \mu(a+r, r) = \mu(a+r, b+r), \tag{4.20}$$

$$\nu(a,b,t) \triangleright \mu(a+r, r) = \nu(a+r, b+r, t). \quad \square \tag{4.21}$$

In the next section we are going to study which of the probability quasi-measures $\mu(p,r)$ and $\nu(p,r,t)$ are actually probability measures. For this purpose we will use some of the the following facts, which are available in literature (see [15, 11, 14, 10, 6, 7]): The class of all compactly supported probability measures on $\mathbb{R}$ is closed under the free, boolean, and monotonic convolution and also under taking the powers $\mu^{\boxplus s}$, $\mu^{\uplus t}$, for $s \geq 1$, $t > 0$. Moreover, the class of probability measures with compact support contained in $[0,\infty)$ is closed under the free, multiplicative free, boolean and monotonic convolution and also under taking the powers $\mu^{\boxplus s}$, $\mu^{\boxtimes s}$ and $\mu^{\uplus t}$ for $s \geq 1$ and $t > 0$.
A probability measure μ on $\mathbb{R}$ (resp. on $[0,\infty)$) is called $\boxplus$-*infinitely divisible* (resp. $\boxtimes$-*infinitely divisible*) if $\mu^{\boxplus t}$ (resp. $\mu^{\boxtimes t}$) is a probability measure for every $t > 0$. If μ has compact support and $r_m(\mu)$ are its free cumulants then μ is $\boxplus$-infinitely divisible if and only if the sequence $\{r_{m+2}(\mu)\}_{m=0}^{\infty}$ is positive definite.

5. Positivity

The aim of this section is to study which of the quasi measures $\mu(p,r)$ and $\nu(p,r,t)$ are actually measures, i.e. for which parameters $p,r,t \in \mathbb{R}$ the corresponding sequence is positive definite. We start with

Theorem 5.1. *If $p \geq 1$, $0 \leq r \leq p$ then $\{A_m(p,r)\}_{m=0}^{\infty}$ is the moment sequence of a probability measure $\mu(p,r)$ with a compact support contained in $[0,\infty)$. If $p \leq 0$, $p-1 \leq r \leq 0$ then $\mu(p,r)$ is a probability measure which is the reflection of $\mu(1-p,-r)$.*

Proof. We know already that $\widetilde{\pi} = \mu(2,1)$ is the free Poisson law (1.1). Then, as was noted in [1], $\widetilde{\pi}$ is $\boxtimes$-infinitely divisible and for $s > 0$ we have $\pi^{\boxtimes s} = \mu(1+s,1)$. Hence if $p \geq 1$ then $\mu(p,1)$ is a probability measure with a compact support contained in $[0,\infty)$. By (2.3) it implies that the sequence $A_m(p,p) = A_{m+1}(p,1)$ is also positive definite, namely we have

$$\int_{\mathbb{R}} f(x)\, d\mu(p,p)(x) = \int_{\mathbb{R}} f(x) x\, d\mu(p,1)(x)$$

for any continuous function f on $\mathbb{R}$. Hence $\mu(p,p)$, $p \geq 1$, is a probability measure with a compact support contained in $[0,\infty)$. For $1 \leq r \leq p$ we apply (4.13) to obtain:

$$\mu(p,r) = \mu(r,r) \boxtimes \mu(p/r,1),$$

which proves the first statement for the sector $1 \leq r \leq p$.
For $r \in (0,1)$ the measure $\mu(1,r)$ is related to the Euler beta function

$$B(a,b) := \int_0^1 x^{a-1}(1-x)^{b-1}\, dx. \tag{5.1}$$

We will use its well known properties: $B(a,1-a) = \frac{\pi}{\sin a\pi}$ and $B(a,b) = \frac{a-1}{a+b-1}B(a-1,b)$. If we define probability measure

$$\mu_r := \frac{\sin \pi r}{\pi} x^{r-1}(1-x)^{-r}\, dx \tag{5.2}$$

on $[0,1]$ then we have

$$\int_{\mathbb{R}} x^m \, d\mu_r(x) = \frac{\sin \pi r}{\pi} B(m+r, 1-r) = \prod_{k=1}^{m} \frac{r+i-1}{i} = A_m(1,r).$$

which means that $\mu(1,r) = \mu_r$. Now for $s \geq 0$ we have

$$\mu(1+rs, r) = \mu(1,r) \boxtimes \mu(1+s,1),$$

which proves the first statement for $(p,r) \in [1,+\infty) \times (0,1)$. It remains to note that $\mu(p,0) = \delta_0$ for every $p \in \mathbb{R}$.
The second statement is a consequence of (4.4). □

We conjecture that the last theorem fully characterizes the set of parameters $p, r \in \mathbb{R}$ for which $\mu(p,r)$ is a measure (apart from the trivial case $\mu(p,0) = \delta_0$). It is easy to check that $A_0(p,r)A_2(p,r) - A_1(p,r)^2 = r(2p-1-r)/2$, hence a necessary condition for positive definiteness of the sequence $A_m(p,r)$ is that $r(2p-1-r) \geq 0$.

Remark. According to Penson and Solomon [12]:

$$\mu(3,1) = \frac{\sqrt[6]{108}\left[2^{1/3}\left(27+3\sqrt{81-12x}\right)^{2/3} - 6x^{1/3}\right]}{12\pi x^{2/3}(27+3\sqrt{81-12x})^{1/3}} \, dx \qquad (5.3)$$

on $[0, 27/4]$. More generally, for $\mu(p,1)$ with $p \in \mathbb{N}$ we refer to [8].

Corollary 5.1. *If either $0 \leq 2r \leq p$, $r+1 \leq p$ or $p \leq 2r+1$, $p \leq r \leq 0$ then $\mu(p,r)$ is $\boxplus$-infinitely divisible.*

Proof. By Theorem 13.16 in [11], a compactly supported probability measure μ, with free cumulants $r_m(\mu)$, is $\boxplus$-infinitely divisible if and only if the sequence $\{r_{m+2}(\mu)\}_{m=0}^{\infty}$ is positive definite. Then it is sufficient to refer to (4.8) and to note that the numbers $A_{m+2}(p-r,r)$ are the moments of the measure $x^2 \, d\mu(p-r,r)(x)$. □

Corollary 5.2. *If $0 \leq r \leq p-1$, $t > 0$ then $\nu(p,r,t)$ is a probability measure with a compact support contained in $[0,+\infty)$. If $p \leq 1+r \leq 0$, $t < 1$ then $\nu(p,r,t)$ is a probability measure which is the reflection of $\nu(1-p,-1-r,1-t)$. In particular, if either $0 \leq r \leq p-1$ or $p \leq 1+r \leq 0$ then the sequence $\left\{\binom{mp+r}{m}\right\}_{m=0}^{\infty}$ is positive definite.*

Proof. For $0 \leq r \leq p-1$, $t > 0$ we apply (4.21) and (4.18):

$$\nu(p,r,t) = \nu(p-r,0,t) \rhd \mu(p,r) = \mu(p-r,1)^{\uplus t} \rhd \mu(p,r)$$

and Theorem 5.1. Then we use (4.5). □

A measure ν on $\mathbb{R}$ is called *symmetric* if $\widehat{\nu} = \nu$. For a probability quasi-measure μ define its *symmetrization* μ^{s} by $M_{\mu^{\mathrm{s}}}(z) := M_\mu\left(z^2\right)$. If μ is a probability measure with support contained in $[0,\infty)$ then μ^{s} is a symmetric measure on $\mathbb{R}$, which satisfies $\int_{\mathbb{R}} f(t^2)\, d\mu^{\mathrm{s}}(t) = \int_{\mathbb{R}} f(t)\, d\mu(t)$ for every compactly supported continuous function on $\mathbb{R}$. Denote by $\mu^{\mathrm{s}}(p,r)$ and $\nu^{\mathrm{s}}(p,r,t)$ the symmetrization of $\mu(p,r)$ and $\nu(p,r,t)$. Then, by (3.4) and (4.9), for the free additive transform we have

$$R_{\mu^{\mathrm{s}}(p,r)}(z) = \mathcal{B}_{p-2r}\left(z^2\right)^r - 1. \tag{5.4}$$

In the same way as Corollary 5.2 one can prove

COROLLARY 5.3. *If $p \geq 1$, $0 \leq r \leq p$ then $\mu^{\mathrm{s}}(p,r)$ is a symmetric probability measure on $\mathbb{R}$. Moreover, if $p - 2r \geq 1$ and $0 \leq 3r \leq p$ then $\mu^{\mathrm{s}}(p,r)$ is $\boxplus$-infinitely divisible.* □

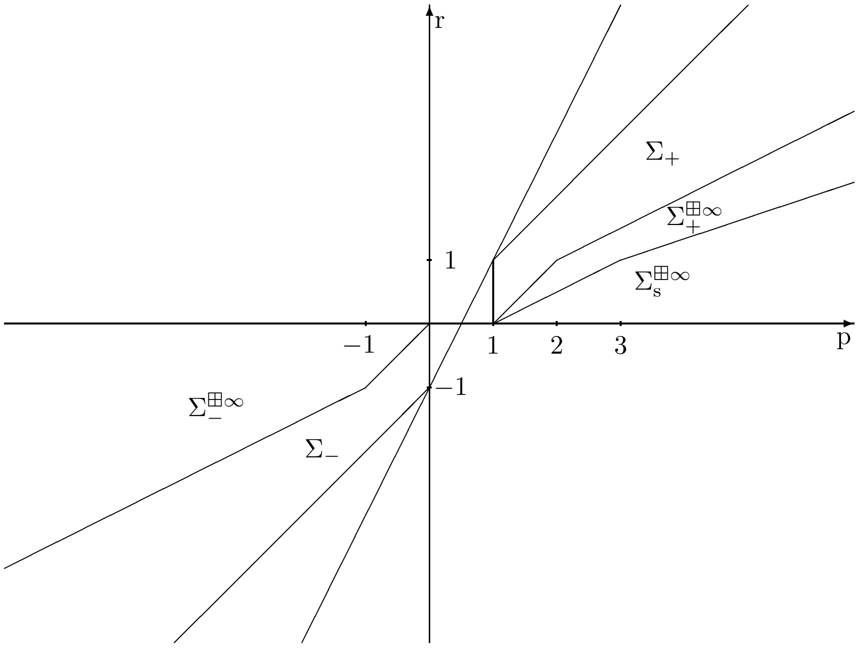
Let us record some formulas:

$$\mu^{\mathrm{s}}(p,1)^{\uplus t} = \nu^{\mathrm{s}}(p,0,t), \tag{5.5}$$

$$\mu^{\mathrm{s}}(a,b) \rhd \mu^{\mathrm{s}}(a+2r,r) = \mu^{\mathrm{s}}(a+2r,b+r), \tag{5.6}$$

$$\nu^{\mathrm{s}}(a,b,t) \rhd \mu^{\mathrm{s}}(a+2r,r) = \nu^{\mathrm{s}}(a+2r,b+r,t). \tag{5.7}$$

5.1. PICTURE FOR $\mu(p,r)$.



Here we illustrate the main results concerning the measures $\mu(p,r)$.

(1) If $\mu(p,r)$ is a probability measure then $r(2p-1-r) \geq 0$ (the right-top and left-bottom sector between the p-axis and the line $r = 2p-1$),
(2) Σ_+ (including $\Sigma_+^{\boxplus\infty}$ and $\Sigma_{\mathrm{s}}^{\boxplus\infty}$): $\mu(p,r)$ is a probability measure with a compact support contained in $[0,\infty)$,
(3) Σ_- (including $\Sigma_-^{\boxplus\infty}$): $\mu(p,r)$ is a probability measure, the reflection of $\mu(1-p,-r)$,
(4) $\Sigma_+^{\boxplus\infty} \cup \Sigma_-^{\boxplus\infty}$ (including $\Sigma_{\mathrm{s}}^{\boxplus\infty}$): $\mu(p,r)$ is $\boxplus$-infinitely divisible,
(5) $\Sigma_{\mathrm{s}}^{\boxplus\infty}$: the symmetrization of $\mu(p,r)$ is $\boxplus$-infinitely divisible.

6. Dilations

For a probability quasi-measure μ we define its *dilation with parameter* $c>0$ by $(\mathrm{D}_c\mu)(x^m) := c^m\mu(x^m)$. Then for the moment generating function we have: $M_{\mathrm{D}_c\mu}(z) = M_\mu(cz)$ and similarly for the free R-transform: $R_{\mathrm{D}_c\mu}(z) = R_\mu(cz)$, while for the S-transform we have $S_{\mathrm{D}_c\mu}(z) = \frac{1}{c}S_\mu(z)$. If μ is proper then we have $(\mathrm{D}_c\mu)(X) = \mu\big(\frac{1}{c}X\big)$ for every Borel subset X of $\mathbb{R}$. In this part we are going to study dilations of the measures $\mu(p,r)$ and $\nu(p,r,t)$ and their limits as the parameter goes to 0.

For $h \geq 0$ and $a,p,r \in \mathbb{R}$ define sequences

$$\binom{a}{m}_h := \frac{1}{m!}\prod_{i=0}^{m-1}(a-ih), \tag{6.1}$$

$$A_m(p,r,h) := \frac{r}{m!}\prod_{i=1}^{m-1}(mp+r-ih), \tag{6.2}$$

with $A_0(p,r,h) := 1$. In particular $A_m(p,r,h) = \frac{r}{mp+r}\binom{mp+r}{m}_h$ whenever $mp+r \neq 0$. Then, for $h \geq 0$ and $p,r,t \in \mathbb{R}$ define probability quasi-measures:

$$\mu(p,r,h)(x^m) := A_m(p,r,h), \tag{6.3}$$

$$\nu(p,r,t,h)(x^m) := \sum_{k=0}^{m} A_{m-k}(p,k(p-h)+r,h)t^k. \tag{6.4}$$

and their moment generating functions $\mathcal{B}_{p,r,h}(z)$ and $\mathcal{D}_{p,r,t,h}(z)$ respectively. Note that if $h>0$ then $A_m(p,r,h) = h^m A_m(p/h,r/h)$ and hence these probability quasi measures can be represented as dilations:

$$\mu(p,r,h) = \mathrm{D}_h\mu(p/h,r/h), \tag{6.5}$$

$$\nu(p,r,t,h) = \mathrm{D}_h\nu(p/h,r/h,t/h). \tag{6.6}$$

Therefore the corresponding moment generating functions are

$$\mathcal{B}_{p,r,h}(z) = \mathcal{B}_{p/h}(hz)^{r/h}, \tag{6.7}$$

$$\mathcal{D}_{p,r,t,h}(z) = \mathcal{D}_{p/h,r/h,t/h}(hz) = \frac{h\mathcal{B}_{p,h+r,h}(z)}{(h-t)\mathcal{B}_{p,h,h}(z)+t}. \tag{6.8}$$

These formulas allow us to derive properties of the probability quasi-measures $\mu(p,r,h)$ and $\nu(p,r,t,h)$ directly from our previous results when $h>0$, and, after taking the limit with $h \to 0$, for $h=0$.

Proposition 6.1. *For $h>0$ and $p,r,t \in \mathbb{R}$*

$$\mathcal{B}_{p,h,h}(z) = 1 + zh\mathcal{B}_{p,p,h}(z), \tag{6.9}$$

$$\log\left(\mathcal{B}_{p,1,0}(z)\right) = z\mathcal{B}_{p,p,0}(z), \tag{6.10}$$

$$\mathcal{D}_{p,r,t,0}(z) = \frac{\mathcal{B}_{p,r,0}(z)}{1-zt\mathcal{B}_{p,p,0}(z)}. \tag{6.11}$$

Proof. First formula is a consequence of (3.3) and (6.7). Then we have

$$\frac{\mathcal{B}_{p,1,h}(z)^h - 1}{h} = \frac{\mathcal{B}_{p,h,h}(z) - 1}{h} = z\mathcal{B}_{p,p,h}(z).$$

Taking the limit with $h \to 0$ we obtain (6.10).
For (6.11) we write use (6.8) and (6.9) to get

$$\frac{1}{h}\big[(h-t)\mathcal{B}_{p,h,h}(z) + t\big] = 1 - (t-h)\frac{\mathcal{B}_{p,h,h}(z) - 1}{h} = 1 - (t-h)z\mathcal{B}_{p,p,h}(z)$$

and then we take limit with $h \to 0$. □

Proposition 6.2. *For $h \geq 0$ and $p, r, s \in \mathbb{R}$ we have*

$$\mathcal{B}_{p-r,s,h}\left(z\mathcal{B}_{p,r,h}(z)\right) = \mathcal{B}_{p,s,h}(z). \qquad \square \tag{6.12}$$

Proposition 6.3. *For $h \geq 0$ and $p, r \in \mathbb{R}$ we have*

$$\nu(p,r,p,h)(x^m) = \binom{mp+r}{m}_h. \tag{6.13}$$

Proof. For $h > 0$ the formula is a consequence of (6.6). Then we take limit with $h \to 0$. □

Proposition 6.4. *For $h \geq 0$ and $p, r, t \in \mathbb{R}$ we have*

$$\mu\widehat{(p,r,h)} = \mu(h-p,-r,h), \tag{6.14}$$

$$\nu\widehat{(p,r,t},h) = \nu(h-p,-h-r,h-t,h). \tag{6.15}$$

Proof. First we note that $A_m(p,r,h)(-1)^m = A_m(h-p,-r,h)$ and then we apply (6.8) and (3.14). □

Proposition 6.5. *For the free transforms we have*

$$R_{\mu(p,r,h)}(z) = \mathcal{B}_{p-r,r,h}(z) - 1 \tag{6.16}$$

$$S_{\mu(p,r,h)}(z) = \frac{(1+z)^{h/r} - 1}{hz}(1+z)^{(r-p)/r} \quad \textit{for } h > 0, \tag{6.17}$$

$$S_{\mu(p,r,0)}(z) = \frac{\log(1+z)}{rz}(1+z)^{(r-p)/r}, \tag{6.18}$$

$$S_{\nu(p,0,t,0)}(z) = \frac{1}{t}e^{\frac{-pz}{t(1+z)}}. \tag{6.19}$$

In particular $\nu(p,0,t,0) = \mathrm{D}_t\left(\nu(1,0,1,0)^{\boxtimes p/t}\right)$.

Proof. Formulas (6.16), (6.17) are consequences of (6.7), (4.11) and (6.12). Therefore, for $h > 0$ we have

$$\mathcal{B}_{p,r,h}\left(\frac{(1+z)^{h/r} - 1}{h}(1+z)^{-p/r}\right) = 1 + z, \tag{6.20}$$

which leads to

$$\mathcal{B}_{p,r,0}\left(\frac{\log(1+z)}{r(1+z)^{p/r}}\right) = 1 + z \tag{6.21}$$

and to (6.18). In particular, substituting $(1+z) \mapsto e^{\frac{pz}{t(1+z)}}$, we have

$$\mathcal{B}_{p,p,0}\left(\frac{z}{t(1+z)}e^{\frac{-pz}{t(1+z)}}\right) = e^{\frac{pz}{t(1+z)}} \tag{6.22}$$

which, combined with (6.11) gives

$$\mathcal{D}_{p,0,t,0}\left(\frac{z}{t(1+z)}e^{\frac{-pz}{t(1+z)}}\right) = \frac{1}{1-\frac{z}{1+z}} = 1+z. \tag{6.23}$$ □

PROPOSITION 6.6. *For $h > 0$ and $p, t \in \mathbb{R}$ we have*

$$\mu(p,h,h)^{\uplus t} = \nu(p,0,th,h), \tag{6.24}$$

$$\nu(p,0,1,0)^{\uplus t} = \nu(p,0,t,0). \tag{6.25}$$

Proof. Since $\mathcal{B}_{p,0,0}(z) = 1$, formula (6.25) is a consequence of (6.11). □

PROPOSITION 6.7. *For $h \geq 0$, $t > 0$, $a, b \in \mathbb{R}$ we have*

$$\mu(a,b,h) \rhd \mu(a+r,r,h) = \mu(a+r,b+r,h), \tag{6.26}$$

$$\nu(a,b,t,h) \rhd \mu(a+r,r,h) = \nu(a+r,b+r,t,h). \tag{6.27}$$ □

PROPOSITION 6.8. *Assume that $h \geq 0$.*
1. If $p \geq h$ and $0 \leq r \leq p$ then $\mu(p,r,h)$ is a probability measure with support contained in $[0,\infty)$. If $p \leq 0$, $p-h \leq r \leq 0$ then $\mu(p,r,h)$ is a probability measure which is the reflection of $\mu(h-p,-r,h)$.
2. If either $0 \leq 2r \leq p$, $r+h \leq p$ or $p \leq 2r+h$, $p \leq r \leq 0$ then $\mu(p,r,h)$ is $\boxplus$-infinitely divisible.
3. If $0 \leq r \leq p-h$, $t > 0$ then $\nu(p,r,t,h)$ is a probability measure with a compact support contained in $[0,+\infty)$. If $p \leq h+r \leq 0$, $t < h$ then $\nu(p,r,t,h)$ is a probability measure which is the reflection of $\nu(h-p,-h-r,h-t,h)$
In particular, if either $0 \leq r \leq p-h$ or $p \leq h+r \leq 0$ then the sequence $\left\{\binom{mp+r}{m}_h\right\}_{m=0}^{\infty}$ is positive definite. □

We conclude with some remarks on the probability measure $\nu_0 := \nu(1,0,1,0)$, for which the moments are $\nu_0(x^m) = \binom{m}{m}_0 = \frac{m^m}{m!}$. From (4.9), (6.19) we have

$$S_{\nu_0}(z) = e^{\frac{-z}{1+z}}, \tag{6.28}$$

$$R_{\nu_0}\left(ze^{\frac{-z}{1+z}}\right) = z, \tag{6.29}$$

$$M_{\nu_0}\left(\frac{z}{1+z}e^{\frac{-z}{1+z}}\right) = 1+z. \tag{6.30}$$

THEOREM 6.1. *The sequence $\left\{\frac{m^m}{m!}\right\}_{m=0}^{\infty}$ is positive definite and the corresponding probability measure ν_0 has compact support contained in $[0,e]$. Moreover, ν_0 is $\boxtimes$-infinitely divisible.*

Proof. First observe that $\lim_{m\to\infty} \sqrt[m]{\frac{m^m}{m!}} = e$, which implies that the support of ν_0 is contained in $[0,e]$. Now we recall (see Theorem 3.7.3 in [2]) that a probability measure μ with support contained in $[0,\infty)$ is $\boxtimes$-infinite divisible if and only if the function $\Sigma_\mu(z) := S_\mu\big(z(1-z)^{-1}\big)$ can be expressed as $\Sigma_\mu(z) =$

$e^{v(z)}$, where $v : \mathbb{C} \setminus [0, \infty) \mapsto \mathbb{C}$ is analytic, satisfies $v(\overline{z}) = \overline{v(z)}$ and maps the upper half-plane $\mathbb{C}^+$ into the lower half-plane $\mathbb{C}^-$. In our case $\Sigma_{\nu_0}(z) = e^{-z}$ and the function $v(z) = -z$ does satisfy these assumptions. □

Let us briefly reconstruct the way we have obtained the measure ν_0. We started with $\widetilde{\pi} = \mu(2, 1, 1)$, the free Poisson measure. Then

$$\mu(p, h, h) = \mathrm{D}_h \mu(p/h, 1, 1) = \mathrm{D}_h \left(\widetilde{\pi}^{\boxtimes \frac{p}{h} - 1} \right),$$

so putting $h = 1/n$, $p = 1$ and using (6.24) with $t = 1/h = n$ we have

$$\left(\mathrm{D}_{\frac{1}{n}} \left(\widetilde{\pi}^{\boxtimes n-1} \right) \right)^{\uplus n} \longrightarrow \nu_0, \qquad \text{with } n \to \infty, \tag{6.31}$$

where the convergence here means that the m-th moment of $\left(\mathrm{D}_{\frac{1}{n}} \left(\widetilde{\pi}^{\boxtimes n-1} \right) \right)^{\uplus n}$ tends to $\frac{m^m}{m!}$. Note also that from (6.29) one can calculate free cumulants of ν_0: $r_1 = 1$, $r_2 = 1$, $r_3 = \frac{1}{2}$, $r_4 = \frac{-1}{3}$. Since $r_4 < 0$, the measure ν_0 is not $\boxplus$-infinitely divisible.

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Almost Proper GIT-Stacks and Discriminant Avoidance

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Abstract. We prove that the classifying stack of an reductive group scheme over a field is very close to being proper. Using this we prove a result about isotrivial families of varieties. Fix a polarized variety with reductive automorphism group. To prove that every isotrivial family with this fibre has a rational section it suffices to prove this when the base is projective, i.e., the discriminant of the family is empty.

1. Introduction

Consider an algebraic stack of the form $[\mathrm{Spec}(k)/G]$ where G is a geometrically reductive group scheme over a field k. It turns out that such a stack is nearly proper, see Proposition 2.5.1. Our proof of this uses ideas very similar to those used by Totaro and Edidin-Graham in their work on equivariant Chow theory. It seems the application of these ideas here is novel.

Next, consider a pair $(V, \mathcal{L})$ consisting of a projective variety V over k and an invertible sheaf. Also, fix an integer $d \geq 1$. We would like to know if every d-dimensional family of polarized varieties $X \to S$, $\mathcal{N} \in \mathrm{Pic}(X)$, all of whose fibres are isomorphic to $(V, \mathcal{L})$, has a rational section. For example this is true if V is a nodal plane cubic.

Theorem 1.0.1. *(See Theorem 2.2.3 which is slightly more general.) Assume $G = Aut(V, \mathcal{L})$ is geometrically reductive. If $X \to S$ has a rational section whenever S is a projective variety of dimension d then there is a rational section whenever S is a quasi-projective variety, provided* $\dim S \leq d$.

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Loosely speaking this means that if you prove the existence of rational sections whenever the discriminant is empty then you prove it in general. For example, it implies that if you are trying to find rational sections of families of polarized homogenous varieties over surfaces then it suffices to do so in the case of families of homogenous varieties over projective nonsingular surfaces. Our proof of this theorem depends on the result on GIT-stacks mentioned above.

In a forthcoming article, joint with Xuhua He, we use this to prove that certain families of polarized homogeneous varieties over surfaces always have rational sections. This is the crucial step in resolving Serre's "Conjecture II" over function fields of surfaces, cf. [Ser02, p. 137], and also gives a proof of the first author's *Period-Index Theorem*, cf. [dJ04], valid in arbitrary characteristic (another proof valid in arbitrary characteristic was proved independently by Max Lieblich, who also proved some beautiful extensions, cf. [Lie08]).

2. Isotrivial families

The title of this section is a little misleading as usually one thinks of an isotrivial family as having finite monodromy. As the reader will see such families are certainly examples to which our discussion applies, but we also allow for a positive dimensional structure group. The families will be isotrivial in the sense that the fibres over a Zariski open will be all isomorphic to a fixed variety V.

2.1. Generalities on Isom. Let U be a base scheme. Let $f : X \to U$ and $g : Y \to U$ be proper, flat morphisms. Let $\mathcal{N}$ be an f-ample invertible sheaf on X, and let $\mathcal{L}$ be a g-ample invertible sheaf on Y. Consider the functor that associates to a scheme $T \to U$ over U the set of pairs (ϕ, α), where $\phi : X_T \to Y_T$ is an isomorphism over T and $\alpha : \phi^*\mathcal{L}_T \to \mathcal{N}_T$ is an isomorphism of invertible sheaves. This functor is representable, see [Gro62, No. 221-19, §4.c], [Gro63, Corollaire 7.7.8], and [LMB00, Théorème 4.6.2.1]. We will call the representing U-scheme $\mathrm{Isom}_U((X,\mathcal{N}),(Y,\mathcal{L}))$.

In fact this U-scheme is affine over U. To see this, it is first convenient to change $\mathcal{L}$ and $\mathcal{N}$. For every integer $N > 0$ there is an obvious morphism

$$\mathrm{Isom}_U((X,\mathcal{N}),(Y,\mathcal{L})) \to \mathrm{Isom}_U((X,\mathcal{N}^N),(Y,\mathcal{L}^N)).$$

It is straightforward to verify that this morphism is finite. Therefore we can reduce to the case that $\mathcal{L}$ and $\mathcal{N}$ are relatively *very ample* and also have vanishing higher direct images. Then the natural map

$$\mathrm{Isom}_U((X,\mathcal{N}),(Y,\mathcal{L})) \to \mathrm{Isom}_U(f_*\mathcal{N}, g_*\mathcal{L})$$

is a closed immersion whose target is clearly affine over U, cf. [Gro63, 7.7.8, 7.7.9].

2.2. Statement of the result. Let k be an algebraically closed field of any characteristic. We assume given a projective scheme V over k and an ample invertible sheaf $\mathcal{L}$ over V. We let $m = \dim V$. We introduce another integer $d \geq 1$ which will be an upper bound for the dimension of the base of our families. We are going to ask the following question: Is it true that for any polarized family of schemes over a $\leq d$-dimensional base whose general fibre is V, there is a rational point on the generic fibre? We make this more precise as follows.

Situation 2.2.1. Here we are given a triple $(K/k, X \to S, \mathcal{N})$, with the following properties: (a) The field K is an algebraically closed field extension of k. (b) The map $X \to S$ is a proper morphism to a projective variety S over K. (c) The dimension of S is at most d. (d) We are given an invertible sheaf $\mathcal{N}$ on X. (e) For a general point $s \in S(K)$ we have $(X_s, \mathcal{N}_s) \cong (V_K, \mathcal{L}_K)$.

The notation $(V_K, \mathcal{L}_K)$ refers to the base change of the pair $(V, \mathcal{L})$ to Spec K. Part (e) means that there exists a nonempty Zariski open $U \subset S$ over which the morphism is flat and such that $(X_s, \mathcal{N}_s) \cong (V_K, \mathcal{L}_K)$ as pairs over K for all $s \in U$. We will see in Lemma 2.3.2 that this implies $\mathrm{Isom}_U((X, \mathcal{N}), (V_U, \mathcal{L}_U))$ is a torsor, hence all geometric fibres of $X \to S$ over U are isomorphic to a suitable base change of V.

Question 2.2.2. Suppose we are in Situation 2.2.1. Is there a rational point on the generic fibre of $X \to S$? In other words: Is $X(K(S))$ not empty?

A natural problem that arises when studying this question is the possibility of bad fibres in the family $X \to S$. Let us define the discriminant Δ of a family $(K/k, X \to S, \mathcal{N})$ as in Situation 2.2.1 as the Zariski closure of the set of points $s \in S(K)$ such that $(X_s, \mathcal{L}_s)$ is not isomorphic to $(V_K, \mathcal{L}_K)$. A priori the codimension of (the closure of) Δ is assumed ≥ 1, and typically it will be 1. In this section we show that it often suffices to answer Question 2.2.2 in cases where the codimension of Δ is bigger, at least as long as we are answering the question for all families.

It is not surprising that the automorphism group G of the pair $(V, \mathcal{L})$ is an important invariant of the situation. The group scheme G has T-valued points which are pairs (ϕ, α), where $\phi : V_T \to V_T$ is an automorphism of schemes over T, and $\alpha : \phi^*\mathcal{L}_T \to \mathcal{L}_T$ is an isomorphism of invertible sheaves. It is representable by Subsection 2.1. The group law is given by $(\phi, \alpha) \cdot (\psi, \beta) = (\phi \circ \psi, \beta \circ \psi^*(\alpha))$. And G is an affine group scheme over k. In the following theorem G°_{red} denotes the reduction of the identity component of G. Note that G°_{red} is a smooth affine group scheme (since k is algebraically closed, and hence perfect).

Theorem 2.2.3. *Fix $(V, \mathcal{L})$ and d as above. Assume that G°_{red} is reductive. If the answer to Question 2.2.2 is yes whenever $\Delta = \emptyset$, then the answer to Question 2.2.2 is yes in all cases.*

The proof has 2 parts: deformation and specialization. The deformation argument proves the following: For every triple $(K/k, X \to S, \mathcal{N})$, there is a dense open subset $U \subset S$ and a deformation of $(X_U \to U, \mathcal{N}|_{X_U})$ to a triple $(K'/k, X' \to S', \mathcal{N}')$ with trivial discriminant. The specialization argument proves the following: Every rational point of the generic fiber of $X' \to S'$ specializes to a rational point of the generic fiber of $X \to S$. Thus Question 2.2.2

has a positive answer for $(K/k, X \to S, \mathcal{N})$ if it has a positive answer for $(K'/k, X' \to S', \mathcal{N}')$.

2.3. A bijective correspondence. To deform the pair $(X_U \to U, \mathcal{N}|_{X_U})$, it is convenient to first convert the pair into a G-torsor over U, deform the torsor, and then convert this back into a triple. This subsection describes how to convert between pairs and G-torsors. As in subsection 2.2, denote by G the automorphism group scheme of $(V, \mathcal{L})$. Following is a quick proof of a well-known result about homogeneous spaces.

Lemma 2.3.1. *Let Γ be a finite type group scheme over k acting on a nonempty, reduced, finite type k-scheme X. If the induced morphism*

$$\Psi : \Gamma \times_{Spec\ k} X \to X \times_{Spec\ k} X, \quad (g, x) \mapsto (g \cdot x, x)$$

is surjective on geometric points, then it is flat so that X is a homogeneous space under Γ. If, moreover, Γ is smooth over k, then also X is smooth over k.

Proof. By [Gro67, Théorème 11.1.1], the set U of points in $\Gamma \times_{\text{Spec } k} X$ at which Ψ is flat is open. The morphism Ψ is equivariant for the $\Gamma \times_{\text{Spec } k} \Gamma$-actions,

$$(\Gamma \times_{\text{Spec } k} \Gamma) \times_{\text{Spec } k} (\Gamma \times_{\text{Spec } k} X) \to \Gamma \times_{\text{Spec } k} X, \ \ (\gamma', \gamma) \cdot (g, x) := (\gamma' g \gamma^{-1}, \gamma \cdot x),$$

$$(\Gamma \times_{\text{Spec } k} \Gamma) \times_{\text{Spec } k} (X \times_{\text{Spec } k} X) \to X \times_{\text{Spec } k} X, \ \ (\gamma', \gamma) \cdot (x', x) := (\gamma' \cdot x', \gamma \cdot x).$$

Therefore U is $(\Gamma \times_{\text{Spec } k} \Gamma)$-invariant. Every invariant subset of $\Gamma \times_{\text{Spec } k} X$ is of the form $\Gamma \times_{\text{Spec } k} V$ for a Γ-invariant subset V of X. Since $X \times_{\text{Spec } k} X$ is reduced, Ψ is flat at every point of $\Gamma \times_{\text{Spec } k} X$ mapping to a generic point of $X \times_{\text{Spec } k} X$. And such points exist by the hypothesis that Ψ is surjective. Therefore U is nonempty, i.e., V is nonempty. Finally, by the hypothesis that Ψ is surjective, the only nonempty, Γ-invariant open subset V of X is $V = X$. Therefore U equals $\Gamma \times_{\text{Spec } k} X$, i.e., Ψ is flat.

Finally, assume that Γ is smooth over k. For any k-point x of X (which exists since X is nonempty), the induced morphism

$$\Psi_x : \Gamma \to X, \quad g \mapsto g \cdot x$$

is flat, since it is the base change of Ψ by the morphism

$$X \mapsto X \times_{\text{Spec } k} X, \ x' \mapsto (x', x).$$

Therefore, by [Gro67, Proposition 17.7.7], X is smooth over k. □

Lemma 2.3.2. *Let U be a k-scheme. Let $(X \to U, \mathcal{N})$ be a pair where $X \to U$ is a flat proper morphism and $\mathcal{N}$ is an invertible sheaf on X. Assume that the geometric fiber of $(X, \mathcal{N})$ over U is isomorphic to the base change of $(V, \mathcal{L})$ for a dense set of geometric points of U. Also assume that U is reduced. Then the scheme $\mathcal{T} := Isom_U((X, \mathcal{N}), (V, \mathcal{L}))$, with its natural G-action, is a G-torsor over U.*

Proof. It suffices to prove that $(X, \mathcal{N})$ is locally in the fppf topology of U isomorphic to the constant family $(V, \mathcal{L}) \times U$. To prove this we need some notation.

Take N so large that $\mathcal{L}^N$ is very ample on V and has vanishing higher cohomology groups. Let $n = \dim \Gamma(V, \mathcal{L}^N)$. A choice of basis of $\Gamma(V, \mathcal{L}^N)$ determines a closed immersion $i : V \to \mathrm{P}^{n-1}$. This determines a point $[i]$ of the Hilbert scheme $\mathrm{Hilb} = \mathrm{Hilb}_{\mathrm{P}^{n-1}/k}$. The smooth algebraic group PGL_n acts on Hilb, and we denote by Z the orbit of $[i]$, which is a locally closed subscheme of Hilb. By Lemma 2.3.1, Z is a smooth scheme and the morphism $\mathrm{PGL}_n \to Z$ associated to any k-point of Z is flat. By construction the pullback of the universal family over Z to PGL_n is canonically isomorphic to $V \times \mathrm{PGL}_n$, and the invertible sheaf $\mathcal{O}(1)$ pulls back to $\mathcal{L}^N \boxtimes \mathcal{O}$.

The question is local on U so we may assume that U is affine. By our choice of N above, the invertible sheaf $\mathcal{N}^N$ is very ample on every fibre of X over U with vanishing higher cohomology groups. Hence after possibly shrinking U we can find a closed immersion $X \to \mathrm{P}^{n-1}_U$ which restricts to the embedding given by the full linear series of $\mathcal{N}^N$ on every geometric fibre. Consider the associated moduli map $m : U \to \mathrm{Hilb}$. Since U is reduced, and since each pair $(X_s, \mathcal{N}_s)$ for a dense set of geometric points s is isomorphic to a base change of $(V, \mathcal{L})$, we see that $m(U) \subset Z$.

This implies there is some surjective flat morphism $U' \to U$ and an U'-isomorphism $X' \cong V \times U'$ with the property that $\mathcal{N}^N$ pulls back to $\mathcal{L}^N$. The fiber product $U' = U \times_Z \mathrm{PGL}_n$ parameterizes points of U together with an autmorphism of $\mathbb{P}^n$ transforming the fiber of X isomorphically to $i(V)$. Since $\mathrm{PGL}_n \to Z$ is surjective and flat, $U' \to U$ is also surjective and flat. To finish, do the same thing for $N+1$ to get some $U'' \to U$. Then over $U''' := U' \times_U U''$ there is an isomorphism of the pullback of $(X, \mathcal{N})$ and the base change of $(V, \mathcal{L})$. This proves the result. □

Conversely, given a left G-torsor $\mathcal{T}$ over U we will construct a flat proper family of varieties $X \to U$ and an invertible sheaf $\mathcal{N}$ on X such that $\mathrm{Isom}_U((X, \mathcal{N}), (V_U, \mathcal{L}_U))$ is isomorphic to $\mathcal{T}$. Of course it will turn out that X equals $(V \times \mathcal{T})/G$ (as an fppf sheaf), but we need to prove this is a scheme.

The structure morphism $\pi : \mathcal{T} \to U$ is a flat surjective morphism of finite type. We are going to descend the constant family $V \times \mathcal{T}$ to U using a descent datum

$$\phi : V \times \mathcal{T} \times_U \mathcal{T} \to V \times \mathcal{T} \times_U \mathcal{T}.$$

Before we describe the descent datum, we recall that the map

$$\Psi : G \times \mathcal{T} \to \mathcal{T} \times_U \mathcal{T}, \quad (g, t) \mapsto (g \cdot t, t)$$

is an isomorphism. Also, let us denote $m : V \times G \to V$ the map $(v, g) \mapsto gv$, where gv denote the natural action of $g \in G$ on $v \in V$. Finally, we take

$$\phi = \mathrm{Id}_V \times \Psi \circ m \times \mathrm{Id}_{\mathcal{T}} \circ (\mathrm{Id}_V \times \Psi)^{-1}.$$

To verify the cocycle condition on $\mathcal{T} \times_U \mathcal{T} \times_U \mathcal{T}$, we can think of ϕ as the map $(v, gt, t) \mapsto (g^{-1}v, gt, t)$. If on $V \times \mathcal{T} \times_U \mathcal{T} \times_U \mathcal{T}$ we have a point (v, g_1g_2t, g_2t, t) then $\mathrm{pr}_{23}^*(\phi)(v, g_1g_2t, g_2t, t) = (g_2v, g_1g_2t, g_2t, t)$ and $\mathrm{pr}_{12}^*(\phi) \circ \mathrm{pr}_{23}^*(\phi)(v, g_1g_2t, g_2t, t) = (g_1g_2v, g_1g_2t, g_2t, t)$ and $\mathrm{pr}_{13}^*(\phi)(v, g_1g_2t, g_2t, t) = ((g_1g_2)v, g_1g_2t, g_2t, t)$. Thus $\mathrm{pr}_{13}^*(\phi) = \mathrm{pr}_{12}^*(\phi) \circ \mathrm{pr}_{23}^*(\phi)$ as desired.

Because all the maps in question lift canonically to the invertible ample sheaf $\mathcal{L}$ this actually defines a descent datum on the pair $(V, \mathcal{L})$ for $\mathcal{T} \to U$. As $\mathcal{L}$ is ample, this descent datum is effective, cf. [Gro62, No. 190, §B.1]. Thus there exists a pair $(X \to U, \mathcal{N})$ over U and an isomorphism $\delta : \mathcal{T} \times_U (X, \mathcal{N}) \to \mathcal{T} \times (V, \mathcal{L})$ such that ϕ equals $\mathrm{pr}_1^*\delta \circ \mathrm{pr}_2^*\delta^{-1}$.

Conclusion 2.3.3. The above constructions give a bijective correspondence between pairs $(X \to U, \mathcal{N})$ and left G-torsors over U in case U is a reduced scheme over k.

Remark 2.3.4. The construction of the family $(X, \mathcal{N})/U$ starting from the torsor $\mathcal{T}$ works more generally when k is a ring as long as: (1) V is a flat projective scheme of finite presentation over k, (2) $\mathcal{L}$ is ample, and (3) the automorphism group scheme $G = \mathrm{Aut}(V, \mathcal{L})$ is flat over k.

2.4. Deforming torsors over a Henselian DVR.

Before proving Theorem 2.2.3, it is useful to say what is known without the hypothesis that G is reductive. We thank Ofer Gabber, Jean-Louis Colliot-Thélène and Max Lieblich for explaining the following proposition.

Proposition 2.4.1. *Let R be a Henselian DVR with residue field k, and let G be a flat separated group scheme of finite type over Spec R. Every torsor for the closed fiber G_k over Spec k is the closed fiber of a torsor for G over Spec R.*

Proof. We first give a proof when G is affine which is all we will use in this paper. The usual proof that every affine group scheme over a field is linear extends to affine, flat group schemes over a DVR, see [ABD$^+$65, Exposé $\mathrm{VI_B}$, Remarque 11.11.1]. Choose a closed immersion $G \to \mathrm{GL}_{n,R}$. The quotient fppf sheaf $X = \mathrm{GL}_{n,R}/G$ is an algebraic space over R, cf. [Art74, Corollary 6.3]. In fact, by [Ana73, Proposition 3.4.2], there exists an fpqc cover Spec $R' \to$ Spec R such that the pullback Spec $R' \times_{\mathrm{Spec}\ R} X$ is a scheme. After base change to R', by [ABD$^+$65, Exposé $\mathrm{VI_A}$, Proposition 9.2] the quotient morphism

$$\mathrm{GL}_{n,R'} \to \mathrm{Spec}\ R' \times_{\mathrm{Spec}\ R} X$$

is faithfully flat, in fact is a G-torsor, and Spec $R' \times_{\mathrm{Spec}\ R} X$ is smooth over R' . But each of these statements (in the category of algebraic spaces) can be checked after faithfully flat base change. Thus also $\mathrm{GL}_{n,R} \to X$ is faithfully flat, in fact a G-torsor, and X is smooth over R. Since $H^1(k, \mathrm{GL}_{n,k}) = \{1\}$, any torsor for G_k is the fibre of the map $\mathrm{GL}_{n,k} \to X_k$ over a k-point of X. Since R is Henselian and since X is smooth, the map $X(R) \to X(k)$ is surjective, and hence every G_k-torsor lifts.

In the general case, i.e., when G is not necessarily affine, we argue as follows. By [LMB00, Prop. 10.13.1], which relies upon Artin's criterion for algebraicity of a stack, the classifying stack BG is an algebraic stack over Spec R. By [LMB00, Thm. 6.3], for each G_k-torsor there exists an affine R-scheme X, a smooth morphism $\phi : X \to BG$, and a k-point x of X such that $\phi(x)$ corresponds to the given G_k-torsor. Denote by t : Spec $R \to BG$ the 1-morphism associated to the trivial G-torsor. Since ϕ is smooth, the base-change pr_R : Spec $R \times_{t,BG,\phi} X \to$ Spec R is smooth. Since t is a surjective flat morphism, the base-change, pr_X : Spec $R \times_{t,BG,\phi} X \to X$ is surjective and flat. By [Gro67, §6.5], it follows that X is smooth over Spec R. Since R is Henselian and X is smooth over Spec R, $X(R) \to X(k)$ is surjective; in particular there is an R-morphism Spec $R \to X$ extending the given k-point of X. The composition of this morphism with ϕ determines a G-torsor over Spec R whose closed fiber is isomorphic to the given G_k-torsor over Spec k. □

Corollary 2.4.2. *Let R be a DVR with residue field k, and let G be a separated, finite type, flat group scheme over Spec R. Let U be a finite type, integral k-scheme, and let $\mathcal{T}_U \to U$ be a G_k-torsor. There exists an integral, flat, quasi-projective R-scheme Y, with nonempty special fibre Y_k, a G-torsor $\mathcal{T} \to Y$, and an open immersion $j : Y_k \to U$ such that $j^*\mathcal{T}_U$ is isomorphic to $\mathcal{T}_k$ as G_k-torsors over Y_k.*

$$\begin{array}{ccccc} \mathcal{T} & \longleftarrow & \mathcal{T}_k & \xrightarrow{j} & \mathcal{T}_U \\ \downarrow & & \downarrow & & \downarrow \\ Y & \longleftarrow & Y_k & \xrightarrow{j} & U \end{array}$$

Proof. First we show there exists an integral, flat, quasi-projective R-scheme Z and an open immersion $j : Z_k \to U$. It suffices to prove this after replacing U by a dense open subset. Thus first replace U by a dense open affine. And then replace U by the regular locus $\mathrm{Reg}(U)$ which is open by [Gro67, Corollaire 6.12.5] and which is dense since it contains the generic point of U (the stalk being a field since U is integral). In particular this implies that $U \to$ Spec k is a local complete intersection morphism, see [Gro67, Proposition 19.3.2]. So after shrinking U some more we may assume that $U =$ Spec $k[x_1, \ldots, x_n]/(f_1, \ldots, f_c)$ is a complete intersection, i.e., $\dim U = n - c$. At this point we simply put $Z =$ Spec $R[x_1, \ldots, x_n]/(F_1, \ldots, F_c)$, where $F_i \in R[\underline{x}]$ lifts f_i.

Define R' to be the local ring of Z at the generic point of Z_k. Then R' is a Noetherian 1-dimensional local ring. Denote by π a uniformizer of R. Clearly, π maps into $\mathfrak{m}_{R'}$ and $R'/\pi R'$ is the function field of Z_k, i.e., the function field of U. Because R' is R-flat, π is a nonzerodivisor. Thus R' is a DVR with residue field $K = k(U)$.

By Proposition 2.4.1, the G_k torsor over $R'/\pi R'$ lifts to a G-torsor $\mathcal{T}^h$ over the Henselization of R'. By a standard limit argument, this lift exists over an étale extension $R' \to R''$ contained in the Henselization of R'. Note that the residue field $R''/\pi R''$ of R'' is still the function field of U. By a standard limit argument, there is an étale morphism $Y \to Z$ such that $Y_k \to Z_k$ is an open immersion and such that R'' is the local ring of Y at the generic point of Y_k. After replacing Y by an open subscheme, there is a G-torsor $\mathcal{T}$ over Y that pulls back to $\mathcal{T}^h$ over R''. We leave it to the reader to see that, after possible shrinking Y again, this torsor satisfies the conditions of the corollary. □

Corollary 2.4.2 above is a weak version of the deformation principle that we will establish later on. The remaining issue is whether there exists a datum $(Y \to \text{Spec } R, \mathcal{T} \to Y, j : Y_K \to U)$ such that the generic fiber of $Y \to \text{Spec } R$ is projective. Presumably this is not always possible, but in case G is reductive we will show that it is.

Corollary 2.4.2 can be used to lift problems in char $p > 0$ to characteristic 0. Suppose that R is a complete discrete valuation ring with algebraically closed residue field k. Let Ω be an algebraic closure of the fraction field of R. We have in mind the case where $\text{char}(k) = p > \text{char}(\Omega) = 0$. Suppose that V_R is a flat projective R scheme, and that $\mathcal{L}_R$ is an ample invertible sheaf over V_R. We assume that V_Ω and V_k are varieties. Let G_R denote the automorphism group scheme of $(V_R, \mathcal{L}_R)$ over R.

Corollary 2.4.3. *Notations and assumptions as above. Fix $d \in \mathbb{N}$. Assume that G_R is flat over R. If the answer to Question 2.2.2 is always "yes" for the pair $(V_\Omega, \mathcal{L}_\Omega)$ then the answer is always "yes" for the pair $(V_k, \mathcal{L}_k)$.*

Proof. Let $(K/k, X \to S, \mathcal{N})$ be a triple as in Situation 2.2.1 for the pair $(V_k, \mathcal{L}_k)$. Let U be the open subscheme of S over which all geometric fibres of $(X, \mathcal{N})$ are isomorophic to the base change of $(V_k, \mathcal{L}_k)$. The construction in Subsection 2.3 gives a corresponding G_K-torsor $\mathcal{T}_U$ over U.

There exists an extension of complete discrete valuation rings $R \subset R'$ such that the induced extension of residue fields is K/k, see [Gro63, Chapitre 0, 10.3.1]. We apply Corollary 2.4.2 to obtain $Y \to \text{Spec } R'$, $\mathcal{T} \to Y$ and $j : Y_K \to U$. According to Conclusion 2.3.3 and Remark 2.3.4 there exists a pair $(X' \to Y, \mathcal{N}')$ over Y whose restriction to Y_K is isomorphic to $(j^*X|_U, j^*\mathcal{N}|_U)$.

Let Ω' be an algebraic closure of the field of fractions $Q(R')$ of R'. Since $R \subset R'$ we may and do assume that $\Omega \subset \Omega'$. Note that we do not know that the geometric fibre $Y_{\Omega'}$ is irreducible. However, our assumptions imply that X' has a $\Omega'(Y')$-valued point for every irreducible component Y' of $Y_{\Omega'}$. To conclude we apply the lemma below. □

Lemma 2.4.4. *Suppose that R is a DVR with algebraically closed residue field K. Let Ω be an algebraic closure of $Q(R)$. Let $Y \to$ Spec R be a flat, finite type morphism, $X \to Y$ a projective morphism and let $\xi \in Y_K$. Assume in addition that (a) ξ is the generic point of an irreducible component C of the scheme Y_K, (b) the scheme Y_K is reduced at ξ, and (c) for every irreducible component Y' of Y_Ω there exists a $\Omega(Y')$-valued point of X. Then X has a $K(C)$-valued point.*

Proof. Note that right from the start we may replace R by its completion, and hence we may assume that R is excellent, cf. [Gro67, Scholie 7.8.3(iii)]. This will guarantee that the integral closure of R in a finite extension of $Q(R)$ is finite over R, cf. [Gro67, Scholie 7.8.3(vi)]. (In fact this is not necessary if the fraction field of R has characteristic 0, cf. [Mat89, Lemma 1, p. 262].)

By hypothesis, and a standard limit argument, there is a section of $X_\Omega \to Y_\Omega$ over a dense open $V \subset Y_\Omega$, say $s : V \to X_\Omega$. By a standard limit argument, there is a finite extension $Q(R) \subset L$ such that V and s are defined over L. Let R' be the integral closure of R in L. Since R is excellent the extension $R \subset R'$ is a finite extension of DVRs. The residue field of R' is isomorphic to K as K is algebraically closed.

By construction the scheme $Y_{R'} = Y \times_R R'$ has special fibre equal to Y_K. The local ring $\mathcal{O}$ of $Y_{R'}$ at ξ is a DVR. This follows from flatness of $Y_{R'}/R'$ and property (b), see proof of 2.4.2. Thus the image of Spec $Q(\mathcal{O}) \to Y_L$ is one of the generic points of Y_L and hence contained in V. Since $X_{R'} \to Y_{R'}$ is proper, we see that $s|_{\mathrm{Spec}\ Q(\mathcal{O})}$ extends to a $\mathcal{O}$-valued point of $X_{R'}$, and in particular we obtain a $\kappa(\xi) = K(C)$-valued point of $(X_K)_{\kappa(\xi)} = X_{K(C)}$ as desired. □

For example this corollary always applies to the case where $(V, \mathcal{L})$ is the pair consisting of a Grassmanian and its ample generator.

2.5. Deforming torsors for a reductive group. Under the additional hypothesis that G is a geometrically reductive linear algebraic group we can prove a stronger version of Corollary 2.4.2. First we prove that BG is proper over k in some approximate sense.

Proposition 2.5.1. *Let G be a geometrically reductive group scheme over the field k. For each integer c, there exists a smooth k-scheme X, a smooth morphism $\phi : X \to BG$, and an open immersion $j : X \to \overline{X}$ such that*

(i) *$\overline{X}$ is a projective k-scheme,*
(ii) *for every infinite field K and every morphism Spec $K \to BG$, there exists a lift Spec $K \to X$ under ϕ.*
(iii) *$\overline{X} - X$ has codimension $\geq c$,*

The proof uses geometric invariant theory to construct $X \subset \bar{X}$. With more care it may be possible to remove the assumption that K is infinite from (ii).

Proof. Step 1. A "nice" projective representation. By definition G is a linear group scheme. Let V be a finite dimensional k-vector space, and let $\rho' : G \to \mathrm{GL}(V)$ be a closed immersion of group schemes. Consider $\rho : G \to \mathrm{SL}(V \oplus k \oplus k)$ defined by $\rho(g) = \mathrm{diag}(\rho'(g), \det(\rho'(g))^{-1}, 1)$ (diagonal blocks). Observe that the intersection of Image(ρ) and $\mathrm{G}_m\mathrm{Id}$ is the trivial group scheme. Thus, without loss of generality, assume ρ is a closed embedding of G into $\mathrm{SL}(V)$ such that Image(ρ) $\cap\, \mathrm{G}_m\mathrm{Id}$ is the trivial group scheme. In other words, the induced morphism of group schemes $\mathbb{P}\rho : G \to \mathrm{PGL}(V)$ is a closed immmersion.

Step 2. Making the "non-free" locus have codimension $\geq c$. Denote the dimension of V by $n > 1$. Let W be a finite-dimensional k-vector space of dimension c. Denote by H the finite-dimensional k-vector space $\mathrm{Hom}(W, \mathrm{Hom}(V,V))$. There is a linear action $\sigma : \mathrm{GL}(V) \times H \to H$, where an element $g \in \mathrm{GL}(V)$ acts on a linear map $h : W \to \mathrm{Hom}(V,V)$ by $\sigma(g,h)(w) = g \circ h(w)$. This restricts to a linear action of G on H.

Step 3. The GIT quotient. The linear action of G on H determines an action of G on the projective space $\mathbb{P}H$ of lines in H. It comes with a natural linearization of the invertible sheaf $L := \mathcal{O}_{\mathbb{P}H}(1)$ so that the action of G on $H^0(\mathbb{P}H, \mathcal{O}(1)) = \mathrm{Hom}(H,k)$ is the dual of ρ. Denote by $\mathbb{P}H^{\mathrm{ss}}$, resp. $\mathbb{P}H^{\mathrm{s}}_{(0)}$, the semistable, resp. properly stable, locus for the action of G on the pair $(\mathbb{P}H, L)$. Denote by $\overline{X}$ the uniform categorical quotient $\mathbb{P}H^{\mathrm{ss}} /\!\!/ G$ and denote by $p : \mathbb{P}H^{\mathrm{ss}} \to \overline{X}$ the quotient morphism. These exist by [MFK94, Thm. 1.10, App. 1.A, App. 1.C]. By the remark on [MFK94, p. 40], $\overline{X}$ is projective. Also, some power of L is the pullback under p of an ample invertible sheaf on $\overline{X}$. Thus (i) is satisfied for $\overline{X}$.

Step 4. A large open subset of $\mathbb{P}H^{\mathrm{ss}}_{(0)}$ which is a G-torsor. For every element $w \in W - \{0\}$, define F_w to be the homogeneous, degree n polynomial on H defined by $F_w(h) = \det(h(w))$. For every $g \in \mathrm{SL}(V)$,

$$\begin{aligned} F_w(\sigma(g,h)) &= \det(\sigma(g,h)(w)) = \det(gh(w)) \\ &= \det(g)\det(h(w)) = \det(h(w)) = F_w(h). \end{aligned}$$

Thus F_w is invariant for the action of $\mathrm{SL}(V)$. Thinking of F_w as an element of $\Gamma(\mathbb{P}H, \mathcal{O}(n))$ it is invariant for the action of G. Denote by $H_w \subset H$, resp. $\mathbb{P}H_w \subset \mathbb{P}H$, the open complement of the zero locus of F_w. By what was said above, $\mathbb{P}H_w$ is contained in $\mathbb{P}H^{\mathrm{ss}}$. The next step is to prove that $\mathbb{P}H_w$ is contained in $\mathbb{P}H^{\mathrm{s}}_{(0)}$, and, in fact, the geometric quotient $\mathbb{P}H_w \to \mathbb{P}H_w/G$ is a G-torsor.

Let W' be a subspace of W such that $W = \mathrm{span}(w) \oplus W'$. Denote by $H' \subset H$ the subspace $H' = \mathrm{Hom}(W', \mathrm{Hom}(V,V))$. There is a morphism

$$q_w : H_w \to \mathrm{GL}(V) \times H', \quad h \mapsto (h(w), h(w)^{-1} h|_{W'}).$$

The morphism q_w is $\mathrm{GL}(V)$-equivariant if we act on $\mathrm{GL}(V) \times H'$ on the first factor only. There is an inverse morphism

$$r_w : \mathrm{GL}(V) \times H' \to H_w$$

sending a pair (g, h') to the unique linear map $W \to \mathrm{Hom}(V,V)$ such that $w \mapsto g$ and $w' \mapsto gh'(w')$ for every $w' \in W'$. Thus, as a scheme with a left $\mathrm{GL}(V)$-action, H_w is isomorphic to $\mathrm{GL}(V) \times H'$. For the same reason, as a scheme with a $\mathrm{PGL}(V)$-action, $\mathbb{P}H_w$ is isomorphic to $\mathrm{PGL}(V) \times H'$. Thus the categorical quotient of $\mathbb{P}H_w$ by the action of G is the induced morphism $\mathbb{P}H_w \to (\mathrm{PGL}(V)/G) \times H'$. Now the categorical quotient $\mathrm{PGL}(V) \to \mathrm{PGL}(V)/G$, which is also a geometric quotient, is a G-torsor, see [ABD+65, Exposé $\mathrm{VI_A}$, Théorème 3.2] or [MFK94, Proposition 0.9]. Thus also the categorical quotient

$\mathbb{P}H_w \to (\mathrm{PGL}(V)/G) \times H'$ is a G-torsor. In particular, the action of G on $\mathbb{P}H_w$ is proper and free so that $\mathbb{P}H_w$ is contained in $\mathbb{P}H^{\mathrm{ss}}_{(0)}$.

Denote $U = \bigcup \mathbb{P}H_w$, where the union is over all $w \in W - \{0\}$. This is a G-invariant open subscheme of $\mathbb{P}H^{\mathrm{s}}_{(0)}$. Therefore there exists a unique open subscheme $X \subset \overline{X}$ such that $p^{-1}(X) = U$. By the last paragraph, $p : \mathcal{T} \to X$ is a G-torsor. Since U is smooth and p is flat, by [Gro67, §6.5] also X is smooth.

Step 5. Lifting K-valued points of BG to X, K infinite. Associated to the G-torsor U over X, there is a 1-morphism $\phi : X \to BG$. There are also morphisms of stacks $[H/G] \to BG$ and $[\mathbb{P}H/G] \to BG$ because $BG = [\mathrm{Spec}\ k/G]$. By construction, X is 2-equivalent to an open substack of $[\mathbb{P}H/G]$ as a stack over BG. The morphism $[\mathbb{P}H/G] \to BG$ is smooth, since $\mathbb{P}H$ is smooth. Hence $X \to BG$ is smooth. For every field K and 1-morphism $\mathrm{Spec}\ K \to BG$, the 2-fibered product $\mathrm{Spec}\ K \times_{BG} [H/G]$ is a K-vector space, and $\mathrm{Spec}\ K \times_{BG} [\mathbb{P}H/G]$ is the associated projective space. Thus $\mathrm{Spec}\ K \times_{BG} [\mathbb{P}H/G] \cong \mathbb{P}^{cn^2-1}$. Finally, $\mathrm{Spec}\ K \times_{BG} X$ is a nonempty open subscheme of $\mathrm{Spec}\ K \times_{BG} [\mathbb{P}H/G]$. Since K is infinite every dense open subset of $\mathbb{P}^{dn^2-1}_K$ contains a K-point. This proves (ii).

Step 6. The codimension of $\overline{X} - X$ is large. Finally, the codimension of $\overline{X} - X$ is at least as large as the codimension of $\mathbb{P}H - U$. Choosing a basis $(w_1, \dots, w_d)$ for W, $\mathbb{P}H - U$ is contained in the common zero locus of $F_{w_1}, \dots, F_{w_c}$, which clearly has codimension c. Therefore $\overline{X} - X$ has codimension at least c in $\overline{X}$. This proves (iii). □

Corollary 2.5.2. *Let the field k and the group scheme G be as in Proposition 2.5.1. Let R be a DVR containing k with residue field K. Let U be a finite type, integral K-scheme, and let $\mathcal{T}_U \to U$ be a G-torsor. There exists a triple $(Y \to \mathrm{Spec}\ R, \mathcal{T} \to Y, j : Y_K \to U)$ as in Corollary 2.4.2 with the additional property that the generic fiber of Y is projective.*

Proof. We may assume that $\dim U > 0$. Let c be an integer larger than $\dim(U)$. Let $(\phi : X \to BG, X \subset \overline{X})$ be as in Proposition 2.5.1. The torsor $\mathcal{T}_U$ corresponds to a 1-morphism $U \to BG$. By condition (ii), the base-change morphism $\mathrm{Spec}\ K(U) \to BG$ lifts to a morphism $\mathrm{Spec}\ K(U) \to X$. (Note that $K(U)$ is infinite since $\dim U > 0$.) After replacing U by a dense open subscheme, this comes from a morphism $f : U \to X$ lifting $U \to BG$. Also, replace U by an open subscheme that is quasi-projective, say a nonempty open affine. Then for some positive integer N, there is a locally closed immersion of K-schemes, $f' : U \to (X \times \mathbb{P}^N_k)_K$ such $\mathrm{pr}_X \circ f'$ equals f. Denote by m the codimension of $f'(U)$ in $(X \times \mathbb{P}^N_k)_K$.

The scheme $(\overline{X} \times \mathbb{P}^N_k)_R$ is flat and projective over $\mathrm{Spec}\ R$. Choose a closed immersion in $\mathbb{P}^M_R$ for some positive integer M. As in the proof of 2.4.2 we will use that the scheme U is a local complete intersection at a general point, and we will use that X is smooth over k. This implies that $f'(U)$ is dense in a component of a complete intersection of $(\overline{X} \times \mathbb{P}^N_k)_K$ in $\mathbb{P}^M_K$. More precisely, for some positive integer e, there exist homogoneous, degree e polynomials $F_1, \dots, F_m$ on $\mathbb{P}^M_K$ such that the scheme $\overline{Y}_K := \mathrm{V}(F_1, \dots, F_m) \cap (\overline{X} \times \mathbb{P}^N_k)_K$ has pure dimension $\dim(U)$ and contains a nonempty open subscheme U' that is an open subscheme of $f'(U)$. Let $\widetilde{F}_1, \dots, \widetilde{F}_c$ be homogeneous, degree e polynomials on $\mathbb{P}^M_R$ such that for every $i = 1, \dots, m$,

$$(*) \qquad \widetilde{F}_i \equiv F_i \pmod{\mathfrak{m}_R}.$$

Denote by $\overline{Y}$ the zero scheme $\mathrm{V}(\widetilde{F}_1, \dots, \widetilde{F}_m) \cap (\overline{X} \times \mathbb{P}^N_k)_R$. Then $\overline{Y}$ is flat over Spec R by Grothendieck's lemma, see [Mat89, Corollary, p. 179]. The closed fiber of $\overline{Y}$ equals $\overline{Y}_K$. Moreover,

$$\dim((\overline{X} - X) \times \mathbb{P}^N_k) - m \leq \dim X - c + N - m = \dim f'(U) - c < 0.$$

It is easy to see that the set of all possible choices of $\widetilde{F}_i$ satisfying $(*)$ forms a Zariski dense set of points in the relevant vector space of degree e polynomials over the field of fractions $Q(R)$ of R. Thus the dimension count shows there exists a choice of $\widetilde{F}_1, \dots, \widetilde{F}_c$ such that $\overline{Y}_{Q(R)}$ does not intersect $\big((\overline{X} - X) \times \mathbb{P}^N_k\big)_{Q(R)}$. In other words, the generic fiber of $\overline{Y} \to \mathrm{Spec}\ R$ is contained in $(X \times \mathbb{P}^N_k)_{Q(R)}$.

Let η be a generic point of $\overline{Y}$ that specializes to the generic point of U'. Replace $\overline{Y}$ by the closure of η, so that now $\overline{Y}$ is integral. (Presumably, a suitable application of Bertini's theorem could be used to replace this step.) Then $\overline{Y}$ is an integral, flat, projective R-scheme, the closed fiber contains U' as an open subscheme, and the generic fiber is contained in Spec $R \times_{\mathrm{Spec}\ k} (X \times \mathbb{P}^N_k)$. Define

$$Y = \overline{Y} - \big(\overline{Y} \times_{\mathrm{Spec}\ R} \mathrm{Spec}\ K - U'\big).$$

This is an integral, flat, quasi-projective R-scheme whose generic fiber is projective. Moreover, Y_K equals U', which admits a dense, open immersion in S. Finally, the projection $\mathrm{pr}_X : Y \to X$, and the 1-morphism $\phi \circ \mathrm{pr}_X : Y \to BG$ determine a G-torsor $\mathcal{T}$ over Y. By construction, the restriction of this G-torsor to U' is isomorphic to the pullback of $\mathcal{T}_U$ by the open immersion, as desired. □

Remark 2.5.3. We remark that we did not claim that the generic fibre of $Y \to$ Spec (R) is geometrically irreducible. Since X is smooth and geometrically irreducible over k, it seems that with a careful choice of the $\widetilde{F}_i$ and some additional arguments one can obtain this property as well having $Y_{Q(R)}$ smooth over $Q(R)$.

Next we deduce a corollary to help prove Theorem 2.2.3. Let k be an algebraically closed field, and let $(V, \mathcal{L})$ be a pair of a projective k-scheme and an ample invertible sheaf. Denote by G/k the group scheme $G = \mathrm{Aut}(V, \mathcal{L})$. Let $(K/k, X \to S, \mathcal{N})$ be as in Situation 2.2.1. Denote by G°_{red} the reduced, connected component of the identity of G.

Corollary 2.5.4. *Notations as above. Let R be a DVR containing k and with residue field K. If G°_{red} is reductive, there exists an integral, flat, quasi-projective R-scheme Y, a projective, flat morphism $f : \widetilde{X} \to Y$, an invertible sheaf $\widetilde{\mathcal{N}}$ on X, and an open immersion $j : Y_K \to S$ such that:*

(i) *every geometric fiber of $(\widetilde{X}, \widetilde{\mathcal{N}})$ over Y equals the base-change of $(V, \mathcal{L})$,*
(ii) *the restriction of $(\widetilde{X}, \widetilde{\mathcal{N}})$ to Y_K is isomorphic to the pullback of $j^*(X, \mathcal{N})$, and*
(iii) *the generic fiber of $Y \to$ Spec R is projective.*

In particular, let S' be an irreducible component of the geometric generic fibre of $Y \to$ Spec R. Then $(\widetilde{X} \to S', \widetilde{\mathcal{N}})$ over R is a triple $(K'/k, X' \to S', \mathcal{N}')$ with empty discriminant.

Proof. The hypothesis that G°_{red} is reductive implies that it is a geometrically reductive group scheme over k by a result of Haboush, see [Hab75] and [MFK94, Appendix 1.A, p. 191]. Note that G°_{red} is a closed normal subgroup scheme of G and that the quotient G/G°_{red} is a finite group scheme. A finite group scheme over k is geometrically reductive, and an extension of geometrically reductive group schemes is reductive, see [Fog69, Exercise, p. 189 and Lemma 5.57, p. 193]. Hence G is geometrically reductive. Thus the result of this Corollary follows from Corollary 2.5.2 above by applying the bijective correspondence of Conclusion 2.3.3. □

Proof of Theorem 2.2.3. Let us start with an arbitrary triple $(K/k, X \to S, \mathcal{N})$. Let $R = K[[t]]$. So R is Henselian, contains k and has residue field K. Let $\widetilde{X} \to Y \to$ Spec R and $\widetilde{\mathcal{N}}$ be as in Corollary 2.5.4. Denote by Ω/k an algebraic closure of the field of fractions $Q(R)$ of R. Let S' be any irreducible component of Y_Ω and let $X' = \widetilde{X}|_{S'}$, $\mathcal{N}' = \widetilde{\mathcal{N}}|_{S'}$. Thus $(\Omega/k, X' \to S', \mathcal{N}')$ is a triple as in Situation 2.2.1. By construction, this has empty discriminant. By hypothesis, the generic fiber of $X' \to S'$ has a $K'(S')$-point. At this point we apply Lemma 2.4.4 to conclude. □

3. Simple applications

As mentioned in the introduction, our main application of these results is to homogeneous spaces over fraction fields, which will appear in a forthcoming article. But in this section we want to indicate some simple applications of Theorem 2.2.3.

3.1. Fermat Hypersurfaces. As a first case we take V a Fermat hypersurface of degree d in $\mathbb{P}^{d^2-1}$

$$V : T_0^d + T_1^d + \dots T_{d^2-1}^d = 0,$$

with $\mathcal{L} = \mathcal{O}_V(1)$, say over the complex numbers $\mathbf{C}$. In this case the group scheme G is an extension of a finite group by $\mathbf{G}_m$ so certainly reductive. Consider the following family with general fibre $(V, \mathcal{L})$ over $\mathbb{P}^2$:

$$(*) \qquad \sum_{0 \leq i,j \leq d-1} X^i Y^j Z^{2d-2-i-j} T_{i+dj}^d = 0,$$

We learned about this family in personal communication with Tom Graber. This family does not have a rational point over $k(\mathbb{P}^2)$. The reader may enjoy finding an elementary proof of this by looking at what it means to have a polynomial solution to the above. We conclude from Theorem 3.1 that there is a smooth projective family over a projective surface with *every* fibre isomorphic to $(V, \mathcal{L})$, without a rational section. We like this example because it is not immediately obvious how to write one down explicitly.

There is another reason why the family given by $(*)$ is interesting. Tsen's theorem asserts that, if $n \geq d^2$ then any degree d hypersurface $X \subset \mathbb{P}^n_F$, where F is the function field of a surface has a rational point. The authors of this paper wonder what the obstruction to the existence of a rational point is in the boundary case, namely degree d in $\mathbb{P}^{d^2-1}$. One guess is that it is a Brauer class, i.e., an element α in the Brauer group of F such that for finite extensions F'/F one has: $X(F') \neq \emptyset \Leftrightarrow \alpha|_{F'} = 0$. However, the example above shows that this is not the case.

Namely, in our example $F = \mathrm{C}(x, y)$ where $x = X/Z$ and $y = Y/Z$. Anand Depokar pointed out that $(*)$ obtains a rational point over $F(\xi)$ where ξ is a dth root of a nonzero polynomial of the form

$$f(x, y) = - \sum_{0 \leq i,j \leq d-1, (i,j) \neq (0,0)} a_{i,j} x^i y^j.$$

(Just take $T_0 = \xi$ and $T_{i+jd} = a_{i,j}^{1/d}$.) Let $C \subset \mathbb{P}^2$ be an irreducible curve, not the line at infinity $Z = 0$. Suppose that α ramifies along C. The ramification data gives a cyclic extension $\mathrm{C}(C) \subset \mathrm{C}(C)[g^{1/d'}]$ of degree d', where $1 < d'|d$. There is a choice of of $a_{i,j}$ such that the rational function $f(x, y)$ restricts to a rational function on C such that both $f|_C$ and $g^{-1}f|_C$ are not d'th powers. (Left to the reader.) Thus the pullback of α to F' is still ramified along the pullback of C to the surface whose function field is $\mathrm{C}(x, y)(\xi)$. Contradiction. Hence C does not exist. However, the only Brauer class on $\mathbb{P}^2$ ramified along a single line is 0.

3.2. Projective spaces. Another case is where we take the pair $(V, \mathcal{L})$ to be $(\mathbf{P}^n, \mathcal{O}(n + 1))$. Note that $\mathcal{O}(n + 1) = \omega_{\mathbf{P}^n}^{-1}$ so the families in question are canonically polarized, and we are just talking about the problem of having nontrivial families of Brauer-Severi varieties. In particular, our theorem reduces the problem of proving the nullity of the Brauer group of a curve to the problem of proving the nonexistence of Brauer-Severi varieties having no rational sections over projective nonsingular curves. As far as we know this is not really helpful, since the proof of Tsen's theorem is pretty straigthforward anyway. However, it illustrates the idea!

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Inheriting the Anti-Specker Property

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Abstract. The antithesis of Specker's theorem from recursive analysis is further examined from Bishop's constructive viewpoint, with particular attention to its passage to subspaces and products. Ishihara's principle BD-**N** comes into play in the discussion of products with the anti-Specker property.

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1 Introduction

This note is set in the framework of BISH—Bishop-style constructive mathematics. For all practical purposes this is mathematics with intuitionistic logic, an appropriate set theory (such as that described in [1, 2]), and dependent choice. We assume some familiarity with standard constructive notions such as *inhabited* and *located*; more on these, and on constructive analysis in general, can be found in [4, 10].

First, we recall that a sequence $(z_n)_{n\geqslant 1}$ in a metric space (Z, ρ) is

- eventually bounded away from the point $z \in Z$ if there exist N and $\delta > 0$ such that $\rho(z, z_n) > \delta$ for all $n \geqslant N$;
- eventually bounded away from the subset X of Z if there exist N and $\delta > 0$ such that $\rho(x, z_n) > \delta$ for all $x \in X$ and all $n \geqslant N$;
- eventually not in X if there exists N such that $z_n \notin X$ for all $n \geqslant N$.

We call a metric space Z a ONE-POINT EXTENSION of a subspace X if $Z = X \cup \{\zeta\}$ for some ζ such that $\rho(\zeta, X) > 0$. Note that the expression "$\rho(\zeta, X) > 0$" is used, without any implication that the distance from ζ to X exists, as shorthand for

$$\exists_r > 0 \forall_{x \in X} (\rho(\zeta, x) > r).$$

If the distance $\rho(x, X)$ exists, we say that X is LOCATED in Z.

In an earlier paper [6], we introduced the following (unrelativised)[1] ANTI-SPECKER PROPERTY for X,

> AS^1_X For some one-point extension Z of X, every sequence in Z that is eventually bounded away from each point of X is eventually not in X,

which expresses the antithesis of Specker's famous theorem of recursion theory [14]. As is shown in [6], AS^1_X is independent of the one-point extension Z with respect to which it is stated. With classical logic, it is equivalent to the sequential compactness of X. Relative to BISH, $\mathrm{AS}^1_{[0,1]}$ is equivalent to Brouwer's fan theorem FT_c for so-called "c-bars"[3]; so it is not unreasonable to regard the anti-Specker property as a serious candidate for the role of constructive substitute for the classical, and clearly nonconstructive, property of sequential compactness.

Now if AS^1_X is to be a decent substitute for a classical compactness property, we would expect it to have inheritance properties like those of the standard constructive notion of compactness (that is, completeness plus total boundedness). Thus we might hope to prove that every inhabited, closed, located subspace of a space with the anti-Specker property would have that same property; that if an inhabited subspace Y of a metric space has the anti-Specker property, then Y is closed and located; and that the product of two spaces with the anti-Specker property has that property. We address such concerns in this paper.[2]

2 Anti-Specker for subspaces

For the proof of our first result we need a surprisingly useful result in constructive analysis, BISHOP'S LEMMA: If Y is an inhabited, complete, located subset of a metric space X, then for each $x \in X$ there exists $y \in Y$ such that if $\rho(x, y) > 0$, then $\rho(x, Y) > 0$ ([4], page 92, Lemma (3.8)).

PROPOSITION 1 *Let X be a metric space with the property AS^1_X, and let Y be an inhabited, complete, located subspace of A. Then AS^1_Y holds.*

[1] There is a more general, *relativised*, anti-Specker property; see [3, 6].

[2] Some related work is found in [6, 7, 9]. For example, Proposition 10 of [9] tells us that the anti-Specker property is preserved by pointwise continuous mappings.

Proof. Fix a one-point extension $Z \equiv X \cup \{\zeta\}$ of X; then $Y \cup \{\zeta\}$ is a one-point extension of Y. Consider a sequence $(w_n)_{n \geqslant 1}$ in $Y \cup \{\zeta\}$ that is eventually bounded away from each point of Y. Given $x \in X$, we show that $(w_n)_{n \geqslant 1}$ is eventually bounded away from x. By Bishop's lemma, there exists $y \in Y$ such that if $\rho(x, y) > 0$, then $\rho(x, Y) > 0$. Choose N and $\delta > 0$ such that $\rho(w_n, y) > \delta$ for all $n \geqslant N$. Either $\rho(x, y) > 0$ or $\rho(x, y) < \delta/2$. In the first case, $\rho(x, Y) > 0$ and therefore $\rho(w_n, x) \geqslant \rho(x, Y) > 0$ for all n. In the second case, $\rho(w_n, x) \geqslant \delta/2$ for all $n \geqslant N$. Thus the sequence $(w_n)_{n \geqslant 1}$ is eventually bounded away from x. Since $x \in X$ is arbitrary, we can apply AS_X^1 to show that $w_n = \zeta$ for all sufficiently large n. Hence AS_Y^1 holds. ■

We can drop the completeness hypothesis in Proposition 1 if, instead, we require Y to be PROXIMINAL in X: that is, for each $x \in X$ there exists $y \in Y$ (a CLOSEST POINT to x in Y) such that $\rho(x, y) = \rho(x, Y)$. For in that case, with Z, ζ, and $(w_n)_{n \geqslant 1}$ as in the above proof, and given $x \in X$, we construct a closest point y to x in Y. There exist $\delta > 0$ and N such that $\rho(w_n, y) > \delta$ for all $n \geqslant N$. Either $\rho(x, y) > \delta/4$ or $\rho(x, y) < \delta/2$. In the first case, $\rho(w_n, x) \geqslant \rho(x, Y) = \rho(x, y) > \delta/4$ for all n; in the second case, $\rho(w_n, x) > \delta/2$ for all $n \geqslant N$. Thus the sequence $(w_n)_{n \geqslant 1}$ is eventually bounded away from x. As before, this leads us to the conclusion that AS_Y^1 holds.

Next, consider an inhabited, located subset Y of a metric space X, such that AS_Y^1 holds. We cannot expect to prove that Y is closed, since the proof of [9] (Proposition 14) shows that the countably infinite, located subspace

$$\{0\} \cup \left\{ \frac{1}{n} : n \geqslant 1 \right\}$$

of $[0, 1]$, whose closedness is an essentially nonconstructive proposition, has the anti-Specker property. However, we can prove that Y has a property classically equivalent to that of being closed. To do so, we need to define the COMPLEMENT of Y (in X):

$$\sim Y \equiv \{x \in X : \forall_{y \in Y} (x \neq y)\},$$

where "$x \neq y$" means "$\rho(x, y) > 0$".

Proposition 2 *Let* X *be a metric space, and* Y *an inhabited, located subset of* X *with the property* AS_Y^1. *Then* $\sim Y$ *is open in* X.

Proof. Let $Z \equiv Y \cup \{\zeta\}$ be any one-point extension of Y. Given x in $\sim Y$, we need only prove that $\rho(x, Y) > 0$; for then the open ball $B(x, \rho(x, Y))$ is contained in $\sim Y$. To that end, we may assume that $\rho(x, Y) < 1/4$. Construct an increasing binary sequence $(\lambda_n)_{n \geqslant 1}$ such that

$$\lambda_n = 0 \Rightarrow \rho(x, Y) < 2^{-n},$$
$$\lambda_n = 1 \Rightarrow \rho(x, Y) > 2^{-n-1}.$$

Note that $\lambda_1 = 0$. If $\lambda_n = 0$, pick $z_n \in Y$ with $\rho(x, z_n) < 2^{-n}$; if $\lambda_n = 1$, set $z_n = \zeta$. Given $y \in Y$, choose N such that $\rho(x, y) > 2^{-N+1}$. If $n \geqslant N$ and $\lambda_n = 0$, then

$$\rho(y, z_n) \geqslant \rho(x, y) - \rho(x, z_n) > 2^{-N+1} - 2^{-n} \geqslant 2^{-N}.$$

It follows that

$$\rho(y, z_n) \geqslant \min\left\{2^{-N}, \rho(\zeta, Y)\right\} \qquad (n \geqslant N).$$

Hence the sequence $(z_n)_{n\geqslant 1}$ is eventually bounded away from each point y of Y. Using AS^1_Y, we see that $z_n = \zeta$, and hence $\lambda_n = 1$, for all sufficiently large n. Thus there exists n such that $\rho(x, Y) > 2^{-n-1}$. ∎

The foregoing proof provides a good example of how to set things up in order to apply the anti-Specker property: create a sequence in the one-point extension such that if the sequence is eventually not in the original space, then the desired property holds. Proofs of this kind can be used widely in constructive analysis in situations where the classical analyst would use sequential compactness.

3 Anti-Specker for products

So much for subspaces. We would also hope that the anti-Specker property will freely pass between a product space and each of its "factors". The passage down from product to factors is relatively straightforward to prove.

PROPOSITION 3 *Let* $X \equiv X_1 \times X_2$ *be the product of two inhabited metric spaces such that* AS^1_X *holds. Then* $\mathrm{AS}^1_{X_k}$ *holds for each* k.

PROOF. For each k, let $Z_k \equiv X_k \cup \{\zeta_k\}$ be a one-point extension of X_k; then $Z \equiv X \cup \{(\zeta_1, \zeta_2)\}$ is a one-point extension of X. Consider any sequence $(y_n)_{n\geqslant 1}$ in Z_1 that is eventually bounded away from each point of X_1. Fixing ξ_2 in X_2, define a sequence $(z_n)_{n\geqslant 1}$ in Z by

$$z_n \equiv \begin{cases} (y_n, \xi_2) & \text{if } y_n \in X_1 \\ \\ (\zeta_1, \zeta_2) & \text{if } y_n = \zeta_1. \end{cases}$$

Consider any $(x_1, x_2) \in X$. There exist N and $\delta > 0$ such that $\rho(y_n, x_1) \geqslant \delta$ for all $n \geqslant N$. Hence

$$\rho(z_n, (x_1, x_2)) \geqslant \min\{\delta, \rho((\zeta_1, \zeta_2), X)\} > 0$$

for each $n \geqslant N$. Thus the sequence $(z_n)_{n\geqslant 1}$ is eventually bounded away from each point of X. By AS^1_X, there exists ν such that $z_n = (\zeta_1, \zeta_2)$, and therefore $y_n = \zeta_1$, for all $n \geqslant \nu$. Hence $\mathrm{AS}^1_{X_1}$, and similarly $\mathrm{AS}^1_{X_2}$, holds. ∎

For a converse of this proposition we recall some notions discussed in [8]. A subset S of $\mathbf{N}$ is said to be PSEUDOBOUNDED if for each sequence $(s_n)_{n\geqslant 1}$ in S, there exists N such that $s_n < n$ for all $n \geqslant N$. Our definition of pseudoboundedness is equivalent to the original one given by Ishihara in [11]; see [13]. In [11], Ishihara introduced the following principle, which has proved of considerable significance in constructive reverse mathematics:

BD-$\mathbf{N}$ Every inhabited, countable, pseudobounded subset of $\mathbf{N}$ is bounded.

THEOREM 4 BISH + BD-$\mathbf{N}$ $\vdash$ *Let* X, Y *be inhabited metric spaces, each having the anti-Specker property. Then the product space* $X \times Y$ *has the anti-Specker property.*

PROOF. Let $X \cup \{\zeta_1\}$ be a one-point extension of X with $\rho(\zeta_1, X) > 1$, and $Y \cup \{\zeta_2\}$ a one-point extension of Y with $\rho(\zeta_2, Y) > 1$. Then $Z \equiv (X \times Y) \cup\{(\zeta_1, \zeta_2)\}$ is a one-point extension of $X \times Y$. Let $(z_n)_{n\geqslant 1}$ be a sequence in Z that is eventually bounded away from each point of $X\times Y$. Given $x \in X$, we aim to prove that the sequence $(\mathrm{pr}_1(z_{n_k}))_{n\geqslant 1}$ is eventually bounded away from x. Fix $\xi_2 \in Y$. If necessary, replacing $(z_n)_{n\geqslant 1}$ by the sequence $(z'_n)_{n\geqslant 1}$, where

$$z'_n \equiv \begin{cases} (x, \xi_2) & \text{if } n = 1 \\ \\ z_{n-1} & \text{if } n > 1, \end{cases}$$

we may assume that $\mathrm{pr}_1(z_1) = x$. Construct a binary mapping α on $\mathbf{N}^+ \times \mathbf{N}^+$ such that

$$\alpha(n,k) = 0 \Rightarrow \rho(\mathrm{pr}_1(z_n), x) < 2^{-k} \text{ and } n \geqslant k,$$
$$\alpha(n,k) = 1 \Rightarrow \rho(\mathrm{pr}_1(z_n), x) > 2^{-k-1} \text{ or } n < k.$$

Then $\alpha(1,1) = 0$, so the countable subset

$$S \equiv \left\{ j \in \mathbf{N}^+ : \exists_n (\alpha(n,j) = 0) \right\}$$

of $\mathbf{N}^+$ is inhabited. We prove that S is pseudobounded. To that end, let $(s_k)_{k\geqslant 1}$ be any sequence in S. By countable choice, there is a mapping $k \rightsquigarrow n_k$ on $\mathbf{N}^+$ such that $\alpha(n_k, s_k) = 0$ for each k. Construct a binary sequence $(\lambda_k)_{k\geqslant 1}$ such that

$$\lambda_k = 0 \Rightarrow s_k < k,$$
$$\lambda_k = 1 \Rightarrow s_k > \frac{k}{2}.$$

Note that if $\lambda_k = 1$, then $n_k \geqslant s_k > k/2$,

$$\rho(\mathrm{pr}_1(z_{n_k}), x) < 2^{-s_k} < 2^{-k/2} < \rho(\zeta_1, X) \leqslant \rho(\zeta_1, x),$$

and so $z_{n_k} \in X \times Y$. Now construct a sequence $(\theta_k)_{k \geqslant 1}$ in $Y \cup \{\zeta_2\}$ as follows: if $\lambda_k = 0$, set $\theta_k = \zeta_2$; if $\lambda_k = 1$, set $\theta_k = \mathrm{pr}_2(z_{n_k}) \in Y$. Given $y \in Y$, compute a positive integer N such that $\rho(z_n, (x, y)) > 2^{-N}$ for all $n \geqslant N$. Consider any $k > 2N$. If $\lambda_k = 0$, then $\rho(\theta_k, y) \geqslant \rho(\zeta_2, Y) > 1 \geqslant 2^{-N}$. If $\lambda_k = 1$, then

$$\rho(z_{n_k}, (x, y)) > 2^{-N} > 2^{-s_k} > \rho(\mathrm{pr}_1(z_{n_k}), x)$$

and therefore

$$\rho(\theta_k, y) = \rho(\mathrm{pr}_2(z_{n_k}), y) = \rho(z_{n_k}, (x, y)) > 2^{-N}.$$

Thus the sequence $(\theta_k)_{k \geqslant 1}$ is eventually bounded away from each point of Y. Since AS_Y^1 holds, there exists K such that $\theta_k = \zeta_2$ for all $k \geqslant K$. It follows that $\lambda_k = 0$, and therefore $s_k < k$, for all such k. This completes the proof that S is pseudobounded.

Applying BD-**N**, we can find J such that $j < J$ for each $j \in S$. If $n \geqslant J$ and $\rho(\mathrm{pr}_1(z_n), x) < 2^{-J-1}$, then $\alpha(n, J) \neq 1$, so $\alpha(n, J) = 0$ and therefore $J \in S$, a contradiction. It follows that if $n \geqslant J$, then $\rho(\mathrm{pr}_1(z_n), x) \geqslant 2^{-J-1}$. Since $x \in X$ is arbitrary, we conclude that the sequence $(\mathrm{pr}_1(z_n))_{n \geqslant 1}$ is eventually bounded away from each point of X. Applying AS_X^1, we obtain N such that $\mathrm{pr}_1(z_n) = \zeta_1$, and therefore $z_n = (\zeta_1, \zeta_2)$, for all $n \geqslant N$. ■

The question remains: is BD-**N** necessary in order to prove

> (*) the product of any two spaces having the anti-Specker property also has that property.

The answer is "no": R. Lubarsky [12] has a topological model in which (*) holds but BD-**N** does not. In a private communication, he has conjectured that the statement (*), which, in view of Theorem 4 and Lubarsky's result, is weaker than BD-**N**, may be independent of BISH; in that case, it would be an interesting and possibly important business to find theorems of analysis that are equivalent, over BISH, to (*).

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Good Reduction of Affinoids on the Lubin-Tate Tower

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Abstract. We analyze the geometry of the tower of Lubin-Tate deformation spaces, which parametrize deformations of a one-dimensional formal module of height h together with level structure. According to the conjecture of Deligne-Carayol, these spaces realize the local Langlands correspondence in their ℓ-adic cohomology. This conjecture is now a theorem, but currently there is no purely local proof. Working in the equal characteristic case, we find a family of affinoids in the Lubin-Tate tower with good reduction equal to a rather curious nonsingular hypersurface, whose equation we present explicitly. Granting a conjecture on the L-functions of this hypersurface, we find a link between the conjecture of Deligne-Carayol and the theory of Bushnell-Kutzko types, at least for certain class of wildly ramified supercuspidal representations of small conductor.

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1 Introduction

Let F be a non-archimedean local field. By the local Langlands correspondence, the irreducible admissible representations of $\mathrm{GL}_h(F)$ are parametrized in a systematic way by h-dimensional representations of the Weil-Deligne group of F. This is established in [LRS93] for fields of positive characteristic and in [Hen00] and [HT01] for p-adic fields. The local Langlands correspondence appears in a geometric context; namely it is realized in the cohomology of the "Lubin-Tate tower", a projective system of deformation spaces of a one-dimensional formal $\mathcal{O}_F$-module of height h, cf. [Dri74]. We refer to this phenomenon as the conjecture of Deligne-Carayol, after the paper [Car90] which contains the

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precise statement of the conjecture. The papers [Car83] and [Car86] prove the conjecture for the case $h = 2$. The complete conjecture of Deligne-Carayol was proved in [Boy99] for fields of positive characteristic and in [HT01] for p-adic fields. Both papers involve embedding F into a global field and appealing to results from the theory of Shimura varieties or Drinfeld modular varieties.

In [Har02], Harris identifies some unsettled problems in the study of the local Langlands correspondence, and top among these is the lack of a purely local proof of the correspondence. Bushnell and Kutzko's theory of types [BK93] parametrizes admissible representations of $\mathrm{GL}_h(F)$ by finite-dimensional characters of open compact-mod-center subgroups. Naturally one hopes to link the parametrization by types to the parametrization by Weil-Deligne representations, so that one might obtain an "explicit local Langlands correspondence." There have been some remarkable efforts in this direction, see [Hen92], [BH05a], [BH05b], [BH06], but these do not seem to interface with the geometric interpretation of the local Langlands correspondence afforded by the conjecture of Deligne-Carayol. Harris asks ([Har02], Question 9) whether the Bushnell-Kutzko types can be realized in the cohomology of analytic subspaces of the Lubin-Tate tower.

In the present effort we demonstrate progress towards an affirmative answer to this question. We construct a family of open affinoids $\mathfrak{Z}$ of the Lubin-Tate tower which have good reduction equal to a hypersurface $\overline{\mathfrak{Z}}$ whose equation we give explicitly, cf. Thm. 1.1 below. The cohomology of these affinoids appears to contain exactly the Bushnell-Kutzko types for those supercuspidal representations whose Weil parameters are of the form $\mathrm{Ind}_{E/F}\,\theta$, where E/F is the unramified extension of degree h and θ is a character of the Weil group of E of conductor $\mathfrak{p}_E^2$, where $\mathfrak{p}_E$ is the maximal ideal of $\mathcal{O}_E$. We refer to these as the unramified supercuspidals of level π^2. The action of the Weil group on $\overline{\mathfrak{Z}}$ is completely transparent. The question of whether the affinoids $\mathfrak{Z}$ really do realize the local Langlands correspondence for such representations is reduced to the calculation of certain L-functions attached to $\overline{\mathfrak{Z}}$, see Conj. 1.6.

It is hoped that this paper will initiate a systematic study of open affinoids with good reduction in the Lubin-Tate tower. The best outcome would be the construction of a semistable model for the Lubin-Tate spaces, using an appropriate covering by open affinoids. This is precisely what is done in [CM06] for the classical modular curves $X_0(Np^3)$, and in [Weib] for Lubin-Tate curves with arbitrary level structure. Then the weight spectral sequence of Rapoport-Zink [RZ80] would compute the cohomology of the Lubin-Tate tower in terms of the reduction of the semistable model. A purely local proof of the conjecture of Deligne-Carayol would then be reduced to the computation of the zeta functions associated to the components of the reduction of the semistable model.

Before stating our main theorem, we introduce some notation. We write $\mathfrak{X}(\pi^n)$, $n \geq 0$, for the system of rigid-analytic spaces comprising the Lubin-Tate tower of deformations of a height h one-dimensional formal $\mathcal{O}_F$-module with Drinfeld level π^n structure; see §2.1 for definitions. Crucial to the analysis are the "canonical points" of $\mathfrak{X}(\pi^n)$ arising from the canonical liftings of Gross [Gro86]:

these are the deformations with extra endomorphisms by the ring of integers in a separable extension E/F. Such a point is defined over the extension $E_n/\hat{E}^{\mathrm{nr}}$ obtained by adjoining the π^n-division points of a formal Lubin-Tate $\mathcal{O}_E$-module of height one.

In our analysis we concentrate on those canonical points for which the associated extension E/F is unramified. We refer to these as *unramified canonical points*. By performing explicit computations with coordinates, we find certain affinoid neighborhoods around each unramified canonical point x which have good reduction. These neighborhoods lie in a space intermediate in the covering $\mathfrak{X}(\pi^2) \to \mathfrak{X}(\pi)$, which we call $\mathfrak{X}(K_{x,2}) = \mathfrak{X}(\pi^2)/K_{x,2}$; for details, see §4.2. Briefly put, x determines an embedding of $\mathcal{O}_F$-algebras $\mathcal{O}_E \hookrightarrow M_n(\mathcal{O}_F)$, and $K_{x,2}$ is the congruence subgroup defined by

$$K_{x,2} = \left\{ g \in 1 + \pi M_n(\mathcal{O}_F) \;\middle|\; \mathrm{Tr}((g-1)\mathcal{O}_E) \subset \mathfrak{p}_F^2 \right\}.$$

Our main result is:

Theorem 1.1. *Assume that F has positive characteristic, with residue field $\mathbf{F}_q$. Let $x \in \mathfrak{X}(\pi^2)$ be an unramified canonical point. There exists an open affinoid neighborhood $\mathfrak{Z}$ of the image of x in $\mathfrak{X}(K_{x,2})$ whose reduction is the smooth hypersurface $\overline{\mathfrak{Z}}$ in the variables $V_1, \dots, V_h$ defined by the equation*

$$\det \begin{pmatrix} V_1^{q^h} - V_1 & V_2^{q^h} - V_2 & V_3^{q^h} - V_3 & \cdots & V_{h-1}^{q^h} - V_{h-1} & V_h^{q^h} - V_h \\ 1 & V_1^q & V_2^q & \cdots & V_{h-2}^q & V_{h-1}^q \\ 0 & 1 & V_1^{q^2} & \cdots & V_{h-3}^{q^2} & V_{h-2}^{q^2} \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 & V_1^{q^{h-1}} \end{pmatrix} = 0.$$

Remark 1.2. Let R be the noncommutative polynomial ring $\mathbf{F}_{q^h}[\tau]/(\tau^{h+1})$, whose multiplication law is given by $\tau\alpha = \alpha^q\tau$, $\alpha \in \mathbf{F}_{q^h}$. Let $A = R \otimes_{\mathbf{F}_{q^h}} \mathbf{F}_{q^h}[V_1, \dots, V_h]$, and let $\Phi\colon A \to A$ be the R-linear endomorphism which sends V_i to V_i^q. Let $g = 1 + V_1\tau + \cdots + V_h\tau^h \in A^\times$; then the coefficient of τ^n in $\Phi^h(g)g^{-1}$ is the determinant appearing in Thm. 1.1. This shows that the hypersurface $\overline{\mathfrak{Z}}$ admits a large group of automorphisms, namely $R^\times$. See §5.3 for an interpretation of this automorphism group in terms of the Jacquet-Langlands correspondence.

Remark 1.3. We expect the condition $\operatorname{char} F > 0$ to be unnecessary. This condition enables us to write down explicit models for universal deformations of formal $\mathcal{O}_F$-modules with level structure, as in §2.2. It may be possible to remove this condition if one is more careful with error terms.

Remark 1.4. In Yoshida's paper [Yos10] the space $\mathfrak{X}(\pi)$ is treated, with no condition on the characteristic of F. In that case one finds an affinoid subdomain of $\mathfrak{X}(\pi) \otimes E_1$ whose reduction is the Deligne-Lusztig variety for $\mathrm{GL}_h(k)$, see §3.5. Based on this calculation, Yoshida proceeds to show that the vanishing cycles of $\mathfrak{X}(\pi)$ realize the local Langlands correspondence for supercuspidal representations "of depth zero".

Remark 1.5. Thm. 1.1 agrees well with our work in [Weib], which gives a detailed description of a stable reduction of the tower $\mathfrak{X}(\pi^n)$ when $h = 2$. In this case the curve $\overline{\mathfrak{Z}}$ is isomorphic over $\mathbf{F}_q$ to a disjoint union of copies of the "Hermitian curve" $Y + Y^q = V^{q+1}$. The Hermitian curve also happens to be isomorphic over $\overline{\mathbf{F}}_q$ to the Deligne-Lusztig curve for $\mathrm{SL}_2(\mathbf{F}_q)$, but this seems to be a coincidence which does not persist for $h > 2$.

In order to apply Thm. 1.1 to the conjecture of Deligne-Carayol, it will be necessary to calculate the compactly supported ℓ-adic cohomology of $\overline{\mathfrak{Z}}$, $\ell \neq p$, as a module for the action of the stabilizer of $\mathfrak{Z}$ in $\mathrm{GL}_2(\mathcal{O}_F)$, which is the group $U^1 = 1 + \pi M_h(\mathcal{O}_F)$. This in turn is equivalent to the calculation of the L-functions of some ℓ-adic sheaves on affine $(h-1)$-space. To wit, let X be the hypersurface over $\mathbf{F}_{q^h}$ whose equation is the one appearing in Thm. 1.1. Then X is an Artin-Schreier cover of $\mathbf{A}^{h-1}/\mathbf{F}_{q^h}$ with Galois group $\mathbf{F}_{q^h}$. For each character ψ of $\mathbf{F}_{q^h}$ with values in $\overline{\mathbf{Q}}_\ell^\times$, let $\mathscr{L}_\psi$ be the corresponding lisse rank one sheaf on $\mathbf{A}^{h-1}$. Then the zeta function $Z(X,t)$ factors as a product of the L-functions $L(\mathbf{A}^{h-1},\mathscr{L}_\psi,t)$ as ψ runs over characters of $\mathbf{F}_{q^h}$.

Conjecture 1.6. *Suppose ψ does not factor through $\mathrm{Tr}_{\mathbf{F}_{q^h}/\mathbf{F}_{q^d}}$ for any proper divisor d of h. Then*

$$L(\mathbf{A}^{h-1},\mathscr{L}_\psi,t) = \left(1 + (-1)^h q^{\frac{h(h-1)}{2}} t\right)^{(-1)^h q^{\frac{h(h-1)}{2}}}.$$

The formula in Conj. 1.6 is striking: it implies that the contribution of the ψ-part of the Euler characteristic $H_c^*(X \otimes \overline{\mathbf{F}}_q, \overline{\mathbf{Q}}_\ell)$ to the quantities $\#X(\mathbf{F}_{q^h}), \#X(\mathbf{F}_{q^{2h}}), \dots$ is the maximum possible under the constraints of the Riemann hypothesis for X. In fact we strongly suspect that X has the maximum number of $\mathbf{F}_{q^{hn}}$-rational points relative to its compactly supported Betti numbers. More to the point, Conj. 1.6 would also imply that $H_c^{h-1}(\mathfrak{Z},\overline{\mathbf{Q}}_\ell)$ realizes the Bushnell-Kutzko types for the unramified supercuspidals of level π^2, and that the action of the Weil group of F on $\mathfrak{Z}$ is in accord with the local Langlands correspondence. We postpone the details of this claim for future work, but see [Weia], §4 and §5 for a comprehensive calculation in the case $h = 2$.

Conj. 1.6 itself can be verified quite easily for $h = 2$, in which case X is a disjoint union of q copies of the Hermitian curve $Y^q + Y = X^{q+1}$: this curve is "maximal" over $\mathbf{F}_{q^2}$ in the sense that it attains the Hasse-Weil bound for the maximum number of $\mathbf{F}_{q^2}$-rational points. Conj. 1.6 can be verified numerically for small values of q and $h > 2$, but unfortunately we cannot give a general proof at this time. The polynomial on the right-hand side of the equation in Thm. 1.1 is degenerate in the sense of [AS89], which frustrates efforts to determine even the degree of the rational function $L(\mathbf{A}^{h-1},\mathscr{L}_\psi,t)$.

The construction of the explicit local Langlands correspondence for unramified supercuspidals appears in [Hen92]. A salient feature of that paper is the discrepancy between two means of passing from a regular character of $E^\times$ to a supercuspidal representation of $\mathrm{GL}_h(F)$. The first construction is the local Langlands correspondence, the second construction is induction from a compact-mod-center subgroup, and the discrepancy, which appears exactly when h is even, manifests as the nontrivial unramified quadratic character of $E^\times$. Granting Conj. 1.6, we arrive at a geometric explanation for this behavior in terms of the eigenvalue of Frobenius on the middle cohomology of the hypersurface X, for these are positive if and only if h is odd. In the subsequent papers [BH05a] and [BH05b] on the explicit local Langlands correspondence there is a systematic treatment of this discrepancy between the two constructions in the "essentially tame" case; we find it very likely that this discrepancy can always be explained by the behavior of Frobenius eigenvalues acting on the cohomology of an open affinoid in the Lubin-Tate tower having good reduction.

We outline our work: In §2, we review the relevant background material from [Dri74] on one-dimensional formal modules and the Lubin-Tate tower. In §3, we impose the condition that $\mathrm{char}\, F > 0$ and establish a functorial construction of top exterior powers of one-dimensional formal $\mathcal{O}_F$-modules which may be of independent interest. The heart of the paper is §4. Given an unramified canonical point x in $\mathfrak{X}(\pi^2)$, we construct a coordinate Y on that space which is invariant under $K_{x,2}$. The coordinate Y is integral on a certain affinoid neighborhood of x in $\mathfrak{X}(\pi^2)$, and the reduction of the minimal polynomial for Y over the ring of integral functions on $\mathfrak{X}(1)$ gives the equation appearing in Thm. 1.1. We conclude in §5 with some basic observations about the hypersurface $\overline{\mathfrak{Z}}$ which we hope will illuminate the formulas in Conj. 1.6 and motivate future work linking Thm. 1.1 to the local Langlands and Jacquet-Langlands correspondences for $\mathrm{GL}_h(F)$.

2 Preliminaries on formal modules

2.1 Definitions

Throughout this paper, F is a local non-archimedean field with ring of integers $\mathcal{O}_F$, uniformizer π and residue field k having cardinality q, a power of the prime p. Let $\mathfrak{p}$ be the maximal ideal of $\mathcal{O}_F$, and let v be the valuation on F, normalized so that $v(\pi) = 1$. We also use v for the unique extension of this valuation to finitely ramified extension fields E of F contained in the completion of the separable closure of F.

Definition 2.1. Let R be a commutative $\mathcal{O}_F$-algebra, with structure map $i\colon \mathcal{O}_F \to R$. A *formal one-dimensional $\mathcal{O}_F$-module* over R is a power series $\mathscr{F}(X,Y) = X + Y + \cdots \in R[\![X,Y]\!]$ which is commutative, associative, admits 0 as an identity, together with a power series $[a]_{\mathscr{F}}(X) \in R[\![X]\!]$ for each $a \in \mathcal{O}_F$ satisfying $[a]_{\mathscr{F}}(X) \equiv i(a)X \pmod{X^2}$ and $\mathscr{F}([a]_{\mathscr{F}}(X), [a]_{\mathscr{F}}(Y)) = [a]_{\mathscr{F}}(\mathscr{F}(X,Y))$.

The addition law on a formal $\mathcal{O}_F$-module $\mathscr{F}$ will usually be written $X +_{\mathscr{F}} Y$. If $\mathscr{F}$ and $\mathscr{F}'$ are two formal $\mathcal{O}_F$-modules, there is an evident notion of an isogeny $\mathscr{F} \to \mathscr{F}'$, and $\mathrm{Hom}(\mathscr{F}, \mathscr{F}')$ has the structure of an $\mathcal{O}_F$-module.

If R is a k-algebra, we either have $[\pi]_{\mathscr{F}}(X) = 0$ or else $[\pi]_{\mathscr{F}}(X) = f(X^{q^h})$ for some power series $f(X)$ with $f'(0) \neq 0$. In the latter case, we say $\mathscr{F}$ has height h over R.

Fix an integer $h \geq 1$. Let Σ be a one-dimensional formal $\mathcal{O}_F$-module over $\overline{k}$ of height h. The functor of deformations of Σ to complete local Noetherian $\hat{\mathcal{O}}_{F^{\mathrm{nr}}}$-algebras is representable by a universal deformation $\mathscr{F}^{\mathrm{univ}}$ over an algebra $\mathcal{A}$ which is isomorphic to the power series ring $\hat{\mathcal{O}}_{F^{\mathrm{nr}}}[\![u_1, \dots, u_{h-1}]\!]$ in $(h-1)$ variables, cf. [Dri74]. That is, if A is a complete local $\hat{\mathcal{O}}_F^{\mathrm{nr}}$-algebra with maximal ideal P, then the isomorphism classes of deformations of Σ to A are given exactly by specializing each u_i to an element of P in $\mathscr{F}^{\mathrm{univ}}$.

2.2 The universal deformation in the positive characteristic case

The results of the previous paragraph take a very simple form in the equal characteristic case. Assume $\mathrm{char}\, F = p$, so that $F = k((\pi))$ is the field of Laurent series over k in one variable, with $\mathcal{O}_F = k[\![\pi]\!]$. Then a model for Σ is given by the simple rules

$$\begin{aligned} X +_\Sigma Y &= X + Y \\ [\zeta]_\Sigma(X) &= \zeta X,\ \zeta \in k \\ [\pi]_\Sigma(X) &= X^{q^h} \end{aligned}$$

The universal deformation $\mathscr{F}^{\mathrm{univ}}$ also has a simple model over $\mathcal{A}$:

$$\begin{aligned} X +_{\mathscr{F}^{\mathrm{univ}}} Y &= X + Y \\ [\zeta]_{\mathscr{F}^{\mathrm{univ}}}(X) &= \zeta X,\ \zeta \in k \\ [\pi]_{\mathscr{F}^{\mathrm{univ}}}(X) &= \pi X + u_1 X^q + \cdots + u_{h-1} X^{q^{h-1}} + X^{q^h}. \end{aligned} \tag{2.2.1}$$

Let $\mathcal{O}_B = \mathrm{End}\,\Sigma$, and let $B = \mathcal{O}_B \otimes_{\mathcal{O}_F} F$. Then B is the central division algebra over F of invariant $1/h$. Let k_h/k be the field extension of degree h: then $\mathcal{O}_B$ is generated by the unramified extension $\mathcal{O}_E = k_h[\![\pi]\!]$ of $\mathcal{O}_K$ of degree h, which acts on Σ in an evident way, together with the endomorphism $\Phi(X) = X^q$. (The relations are $\Phi^h = \pi$ and $\Phi\zeta = \zeta^q\Phi$, $\zeta \in k_h$.) Inasmuch as $\mathcal{A} = \hat{\mathcal{O}}_F^{\mathrm{nr}}[\![u_1, \dots, u_{h-1}]\!]$ is the moduli space of deformations of Σ, the automorphism group $\mathrm{Aut}\,\Sigma = \mathcal{O}_B^\times$ acts naturally on $\mathcal{A}$. It is natural to ask how $\mathcal{O}_B^\times$ acts on the level of coordinates. The action of an element $\zeta \in k_n^\times$ is simple enough: $\zeta(u_i) = \zeta^{q^i-1}u_i$, $i = 1, \dots, h-1$. On the other hand the action of an element such as $1 + \Phi \in \mathcal{O}_B^\times$ seems difficult to give explicitly.

2.3 Moduli of deformations with level structure

Let A be a complete local $\mathcal{O}_F$-algebra with maximal ideal M, and let $\mathscr{F}$ be a one-dimensional formal $\mathcal{O}_F$-module over A, and let $h \geq 1$ be the height of

$\mathscr{F} \otimes A/M$.

Definition 2.2. Let $n \geq 1$. A *Drinfeld level π^n structure* on $\mathscr{F}$ is an $\mathcal{O}_F$-module homomorphism $\phi\colon (\pi^{-n}\mathcal{O}_F/\mathcal{O}_F)^{\oplus h} \to M$ for which the relation

$$\prod_{x \in (\mathfrak{p}^{-1}/\mathcal{O}_F)^{\oplus h}} (X - \phi(x)) \,\Bigg|\, [\pi]_{\mathscr{F}}(X)$$

holds in $A[\![X]\!]$. If ϕ is a Drinfeld level π^n structure, the images under ϕ of the standard basis elements $(\pi^{-n}, 0, \dots, 0), \dots, (0, 0, \dots, \pi^{-n})$ of $(\mathfrak{p}^{-n}/\mathcal{O}_F)^{\oplus h}$ form a *Drinfeld basis* of $\mathscr{F}[\pi^n]$.

Fix a formal $\mathcal{O}_F$-module Σ of height h over $\overline{k}$. Let A be a noetherian local $\hat{\mathcal{O}}_F^{\mathrm{nr}}$-algebra such that the structure morphism $\hat{\mathcal{O}}_F^{\mathrm{nr}} \to A$ induces an isomorphism between residue fields. A *deformation* of Σ with level π^n structure over A is a triple $(\mathscr{F}, \iota, \phi)$, where $\iota\colon \mathscr{F} \otimes \overline{k} \to \Sigma$ is an isomorphism of $\mathcal{O}_F$-modules over $\overline{k}$ and ϕ is a Drinfeld level π^n structure on $\mathscr{F}$.

Proposition 2.3. *[Dri74] The functor which assigns to each A as above the set of deformations of Σ with Drinfeld level π^n structure over A is representable by a regular local ring $\mathcal{A}(\pi^n)$ of relative dimension $h-1$ over $\hat{\mathcal{O}}_F^{\mathrm{nr}}$. Let $X_1^{(n)}, \dots, X_h^{(n)} \in \mathcal{A}(\pi^n)$ be the corresponding Drinfeld basis for $\mathscr{F}^{\mathrm{univ}}[\pi^n]$; then these elements form a set of regular parameters for $\mathcal{A}(\pi^n)$.*

There is a finite injection of $\hat{\mathcal{O}}_F^{\mathrm{nr}}$-algebras $\mathcal{A}(\pi^n) \to \mathcal{A}(\pi^{n+1})$ corresponding to the obvious degeneration map of functors. We therefore may consider $\mathcal{A}(\pi^n)$ as a subalgebra of $\mathcal{A}(\pi^{n+1})$, with the equation $[\pi]_u\left(X_i^{(n+1)}\right) = X_i^{(n)}$ holding in $\mathcal{A}(\pi^{n+1})$.

Let $X(\pi^n) = \operatorname{Spf} \mathcal{A}(\pi^n)$, so that $X(\pi^n)$ is a formal scheme of relative dimension $h-1$ over $\operatorname{Spf} \hat{\mathcal{O}}_F^{\mathrm{nr}}$. Let $\mathfrak{X}(\pi^n)$ be the generic fiber of $X(\pi^n)$; then $\mathfrak{X}(\pi^n)$ is a rigid analytic variety. The coordinates $X_i^{(n)}$ are then analytic functions on $\mathfrak{X}(\pi^n)$ with values in the open unit disc. We have that $\mathfrak{X}(1)$ is the rigid-analytic open unit polydisc of dimension $h-1$.

The group $\mathrm{GL}_h(\mathcal{O}_F/\pi^n\mathcal{O}_F)$ acts on the right on $\mathfrak{X}(\pi^n)$ and on the left on $\mathcal{A}(\pi^n)$. The degeneration map $\mathfrak{X}(\pi^n) \to \mathfrak{X}(1)$ is Galois with group $\mathrm{GL}_h(\mathcal{O}_F/\pi^n\mathcal{O}_F)$. For an element $M \in \mathrm{GL}_h(\mathcal{O}_F/\pi^n\mathcal{O}_F)$ and an analytic function f on $\mathfrak{X}(\pi^n)$, we write $M(f)$ for the translated function $z \mapsto f(zM)$. When f happens to be one of the parameters $X_i^{(n)}$, there is a natural definition of $M\left(X_i^{(n)}\right)$ when $M \in M_h(\mathcal{O}_F/\pi^n\mathcal{O}_F)$ is an arbitrary matrix: if $M = (a_{ij})$, then

$$M\left(X_i^{(n)}\right) = [a_{i1}]_{\mathscr{F}^{\mathrm{univ}}}\left(X_1^{(n)}\right) +_{\mathscr{F}^{\mathrm{univ}}} \cdots +_{\mathscr{F}^{\mathrm{univ}}} [a_{ih}]_{\mathscr{F}^{\mathrm{univ}}}\left(X_h^{(n)}\right). \quad (2.3.1)$$

3 Determinants

A natural first question in the study of the Lubin-Tate tower $\mathfrak{X}(\pi^n)$ is to compute its zeroth cohomology; *i.e.* to determine its geometrically connected components along with the appropriate group actions. This question is answered completely by Strauch in [Str08b]. Let LT be a one-dimensional formal $\mathcal{O}_F$-module over $\hat{\mathcal{O}}_{F^{\mathrm{nr}}}$ for which $\mathrm{LT}\otimes\overline{k}$ has height one. Let $F_0 = \hat{F}^{\mathrm{nr}}$, and for $n \geq 1$, let $F_n = F_0(\mathrm{LT}[\pi^n])$ be the classical Lubin-Tate extension. Let $\chi\colon \mathrm{Gal}(F_n/F_0) \to (\mathcal{O}_F/\pi^n\mathcal{O}_F)^\times$ be the isomorphism of local class field theory, so that $\mathrm{Gal}(F_n/F_0)$ acts on $\mathrm{LT}[\pi^n]$ through χ. Finally, let $\mathfrak{X}_{\mathrm{LT}}(\pi^n)$ be the (zero-dimensional) space of deformations of $\mathrm{LT}\otimes\overline{k}$ with Drinfeld π^n structure, so that $\mathfrak{X}_{\mathrm{LT}}(\pi^n)(F_n)$ is the set of bases for $\mathrm{LT}[\pi^n](F_n)$ as a free $(\mathcal{O}_F/\pi^n\mathcal{O}_F)$-module of rank one. We now paraphrase [Str08b], Thm. 4.4 in the context of the rigid-analytic spaces $\mathfrak{X}(\pi^n)$.

Theorem 3.1. *The geometrically connected components of $\mathfrak{X}(\pi^n)$ are defined over F_n, and there is a bijection*

$$\pi_0(\mathfrak{X}(\pi^n)\otimes F_n) \xrightarrow{\sim} \mathfrak{X}_{\mathrm{LT}}(\pi^n)(F_n).$$

Under this bijection, the action of an element (g, b, τ) in $\mathrm{GL}_h(\mathcal{O}_F)\times\mathcal{O}_B^\times\times \mathrm{Gal}(F_n/F_0)$ on $\mathfrak{X}_{\mathrm{LT}}(\pi^n)(F_n)$ is through the character

$$(g, b, \tau) \mapsto \det(g)\,\mathrm{N}_{B/F}(b)^{-1}\chi(\tau)^{-1} \in (\mathcal{O}_F/\pi^n\mathcal{O}_F)^\times. \tag{3.0.2}$$

(In [Str08b], $\pi_0(\mathfrak{X}(\pi^n)\otimes \mathbf{C}_\pi)$ is identified with $\pi_0(\mathrm{Spec}(F_n\otimes_{F_0}\mathbf{C}_\pi))$, where $\mathbf{C}_\pi$ is the completion of a separable closure of F. But this latter π_0, being the set of F_0-linear embeddings of F_n into $\mathbf{C}_\pi$, is the same as the set of bases for $\mathrm{LT}[\pi^n](\mathbf{C}_\pi)$. Thus Thm. 3.1 carries the same content as the theorem cited in [Str08b].)

As noted in the introduction to [Str08b], Thm. 3.1 suggests a determinant functor $\mathscr{F}\mapsto\Lambda^h\mathscr{F}$ assigning to each deformation $\mathscr{F}$ of Σ a deformation $\Lambda^h\mathscr{F}$ of $\mathrm{LT}\otimes\overline{k}$. This functor would of course identify the top exterior power of the Tate module $T(\mathscr{F})$ with $T(\Lambda^h\mathscr{F})$. In this section we provide just such a determinant functor *in the case of equal characteristic*, taking advantage of the explicit model of the universal deformation $\mathscr{F}^{\mathrm{univ}}$ described in §2.2. More precisely we prove:

Theorem 3.2. *Assume* $\mathrm{char}\, F > 0$. *For each $n \geq 1$ there exists a morphism*

$$\mu_n\colon \mathscr{F}^{univ}[\pi^n]\times\cdots\times\mathscr{F}^{univ}[\pi^n] \to \mathrm{LT}[\pi^n]\otimes\mathcal{A}$$

of group schemes over $\mathcal{A} = \hat{\mathcal{O}}_{F^{\mathrm{nr}}}[\![u_1,\dots,u_{h-1}]\!]$ which is $\mathcal{O}_F$-multilinear and alternating, and which satisfies the following properties:

1. *The maps μ_n are compatible in the sense that*

$$\mu_n([\pi]_{\mathscr{F}^{\mathrm{univ}}}(X_1),\dots,[\pi]_{\mathscr{F}^{\mathrm{univ}}}(X_h)) = \mu_{n-1}(X_1,\dots,X_h)$$

   for $n \geq 2$.

2. *If $X_1,\dots,X_h$ are sections of $\mathscr{F}^{\mathrm{univ}}[\pi^n]$ over an $\mathcal{A}$-algebra R which form a Drinfeld level π^n structure, then $\mu_n(X_1,\dots,X_h)$ is a Drinfeld level π^n structure for $\mathrm{LT}[\pi^n]\otimes R$.*

Remark 3.3. It is also possible to show that μ_n transforms the action of $\mathrm{GL}_h(\mathcal{O}_F)\times\mathcal{O}_B^\times\times\mathrm{Gal}(F_n/\hat{F}^{\mathrm{nr}})$ on $\mathscr{F}^{\mathrm{univ}}[\pi^n]\times\cdots\times\mathscr{F}^{\mathrm{univ}}[\pi^n]$ into the character defined in Eq. (3.0.2), but we will not be needing this.

The proof of Thm. 3.2 will occupy §3.1 and §3.3. Up to isomorphism there is only one formal $\mathcal{O}_F$-module LT whose reduction has height one, so we are free to choose a model for it. For the remainder of the paper, LT will denote the formal $\mathcal{O}_F$-module over $\hat{\mathcal{O}}_{F^{\mathrm{nr}}}$ with operations

$$\begin{aligned} X +_{\mathrm{LT}} Y &= X+Y \\ [\alpha]_{\mathrm{LT}}(X) &= \alpha X,\ \alpha\in k \\ [\pi]_{\mathrm{LT}}(X) &= \pi X + (-1)^{h-1}X^q. \end{aligned}$$

3.1 Determinants of level π structures

First define the polynomial in h variables

$$\mu(X_1,\dots,X_h)=\det\left(X_i^{q^j}\right)\in k[X_1,\dots,X_h]$$

(the exponent j ranges from 0 to $h-1$). Then μ is a k-linear alternating form, known as the Moore determinant, cf. [Gos96], Ch. 1. We will need two simple identities involving μ. The first is

$$\prod_{0\neq a\in k^h}(a_1X_1+\cdots+a_hX_h)=(-1)^h\mu(X_1,\dots,X_h)^{q-1}, \tag{3.1.1}$$

in which the product runs over nonzero vectors $a=(a_1,\dots,a_h)$ in k^h. Second, there is the identity

$$[\pi]_{\mathrm{LT}}(\mu(X_1,\dots,X_n))=\det\left([\pi]_{\mathscr{F}^{\mathrm{univ}}}(X_i)\,\middle|\,X_i^q\,\middle|\,\cdots\,\middle|\,X_i^{q^{h-1}}\right)_{1\le i\le h}, \tag{3.1.2}$$

valid in $\mathcal{A}[X_1,\dots,X_n]$. This is easily seen by expanding the first column of the matrix according to Eq. (2.2.1).

Lemma 3.4. *If $X_1,\dots,X_h$ are sections of $\mathscr{F}^{\mathrm{univ}}[\pi]$, then $\mu(X_1,\dots,X_h)$ is a section of* $\mathrm{LT}[\pi]$. *If the X_i form a Drinfeld basis for $\mathscr{F}^{\mathrm{univ}}[\pi]$, then $\mu(X_1,\dots,X_h)$ constitutes a Drinfeld basis for* $\mathrm{LT}[\pi]$.

Proof. Suppose $X_1,\dots,X_h$ are sections of $\mathscr{F}^{\mathrm{univ}}[\pi]$ over an $\mathcal{A}$-algebra R. Then the claim that $\mu(X_1,\dots,X_h)$ is annihilated by $[\pi]_{\mathrm{LT}}$ follows from Eq. (3.1.2). Now assume that $X_1,\dots,X_h$ is a Drinfeld basis for $\mathscr{F}^{\mathrm{univ}}[\pi]$. This means that

$$\prod_{a\in k^h}(T-(a_1X_1+\cdots+a_hX_h))\ \text{divides}\ [\pi]_{\mathscr{F}^{\mathrm{univ}}}(T)$$

in $R[\![T]\!]$, hence in $R[T]$. Since $[\pi]_{\mathscr{F}^{\text{univ}}}(T)$ is monic, these polynomials are equal:

$$\prod_{a\in k^h}(T-(a_1X_1+\cdots+a_hX_h)) = \pi T+u_1T^q+\cdots+u_{h-1}T^{q^{h-1}}+T^{q^h} \quad (3.1.3)$$

Equating coefficients of T and using Eq. (3.1.1) shows that

$$\mu(X_1,\dots,X_h)^{q-1}=(-1)^h\pi.$$

On the other hand,

$$\prod_{a\in k}(T-a\mu(X_1,\dots,X_h)) = T^q-\mu(X_1,\dots,X_h)^{q-1}T=(-1)^{h-1}[\pi]_{\mathrm{LT}}(T),$$

which shows that $\mu(X_1,\dots,X_h)$ forms a Drinfeld basis for $\mathrm{LT}[\pi]\otimes R$. □

3.2 Good reduction of an affinoid in $\mathfrak{X}(\pi)$

In this interlude we find an affinoid in $\mathfrak{X}(\pi)$ whose reduction is the Deligne-Lusztig variety for $\mathrm{GL}_h(k)$. This is nothing new in light of [Yos10], Prop. 6.15, but it will give a flavor of the corresponding calculation for $\mathfrak{X}(\pi^2)$.

Proposition 3.5. *There is an isomorphism of local $\hat{\mathcal{O}}_{F^{nr}}$-algebras*

$$\frac{\hat{\mathcal{O}}_{F^{nr}}[\![X_1,\dots,X_h]\!]}{\mu(X_1,\dots,X_h)^{q-1}-(-1)^h\pi}\xrightarrow{\sim}\mathcal{A}(\pi)$$

carrying X_i onto $X_i^{(1)}$.

Proof. Let $\mathcal{A}(\pi)'=\hat{\mathcal{O}}_{F^{\mathrm{nr}}}[\![X_1,\dots,X_h]\!]/(\mu(X_1,\dots,X_h)^{q-1}-(-1)^h\pi)$. By Lemma 3.4 there is unique homomorphism $\mathcal{A}(\pi)'\to\mathcal{A}(\pi)$ of $\hat{\mathcal{O}}_{F^{\mathrm{nr}}}$-algebras carrying X_i onto $X_i^{(1)}$. Since the $X_i^{(1)}$ form a system of regular local parameters of $\mathcal{A}(\pi)$, this homomorphism is surjective. The algebra $\mathcal{A}(\pi)$ is a Galois extension of $\mathcal{A}$ with group $\mathrm{GL}_h(k)$. But we can also furnish $\mathcal{A}(\pi)'$ with the structure of an $\mathcal{A}$-algebra, by identifying $u_i\in\mathcal{A}$ with the coefficient of T^{q^i} on the left-hand side of Eq. (3.1.3). Then $\mathcal{A}(\pi)'$ becomes a Galois extension of $\mathcal{A}$ with group $\mathrm{GL}_h(k)$ as well, and the homomorphism $\mathcal{A}(\pi)'\to\mathcal{A}(\pi)$ respects the $\mathcal{A}$-algebra structure. We conclude that $\mathcal{A}(\pi)'\to\mathcal{A}(\pi)$ is an isomorphism. □

Now let E/F be the unramified extension of degree h, and let E_1/E^{nr} be the extension obtained by adjoining a root ϖ of $X^{q^h-1}-(-1)^h\pi$. Then E_1/E^{nr} is totally tamely ramified of degree q^h-1. Let $\mathfrak{X}(1)^{\mathrm{ts}}\subset\mathfrak{X}(1)\otimes E_1$ be the affinoid polydisc defined by the conditions

$$v(u_i)\geq v(\varpi^{q^h-q^i})=\frac{q^h-q^i}{q^h-1}$$

The notation is borrowed from [CM06]: This is exactly the domain on which $\mathscr{F}^{\mathrm{univ}}[\pi]$ admits no canonical subgroups; *i.e.* where $\mathscr{F}^{\mathrm{univ}}$ is "too supersingular". Whenever $\mathscr{F}$ is a deformation of Σ lying in $\mathfrak{X}(1)^{\mathrm{ts}}$, all nonzero roots of $\mathscr{F}[\pi]$ have valuation equal to $v(\varpi)$. By applying the change of variables $X_i = \varpi V_i$ to Prop. 3.5 we find:

Theorem 3.6. *The preimage of $\mathfrak{X}(1)^{\mathrm{ts}}$ in $\mathfrak{X}(\pi)\otimes E_1$ has reduction isomorphic to the smooth affine hypersurface over $\overline{k}$ with equation $\mu(V_1,\dots,V_h)^{q-1}=1$.*

3.3 Determinants of structures of higher level.

Now let $n\geq 1$, and suppose $X_1,\dots,X_h$ are sections of $\mathscr{F}^{\mathrm{univ}}[\pi^n]$. We write $[\pi^a]_u(X)$ as an abbreviation for $[\pi^a]_{\mathscr{F}^{\mathrm{univ}}}(X)$. We define the form μ_n by

$$\mu_n(X_1,\dots,X_h)=\sum_{(a_1,\dots,a_h)}\mu\left([\pi^{a_1}]_u(X_1),\dots,[\pi^{a_h}]_u(X_h)\right),$$

where the sum runs over tuples of integers $(a_1,\dots,a_h)$ with $0\leq a_i\leq n-1$ whose sum is $(h-1)(n-1)$. It is clear that μ_n is k-multilinear and alternating in $X_1,\dots,X_h$. Before proving that μ_n is $\mathcal{O}_F$-linear, we will show:

Proposition 3.7. *For sections $X_1,\dots,X_h$ of $\mathscr{F}^{\mathrm{univ}}[\pi^n]$, we have*

$$[\pi]_{\mathrm{LT}}(\mu_n(X_1,\dots,X_h))=\mu_{n-1}([\pi]_u(X_1),\dots,[\pi]_u(X_h)).$$

In particular $\mu_n(X_1,\dots,X_h)$ is a section of the group scheme $\mathrm{LT}[\pi^n]$.

Proof. Let $a=(a_1,\dots,a_h)$ be a tuple of nonnegative integers. Write $[\pi^a](X)$ for the tuple $([\pi^{a_1}]_u(X_1),\dots,[\pi^{a_h}]_u(X_h))$. Applying Eq. (3.1.2) we find

$$\begin{aligned}[\pi]_{\mathrm{LT}}(\mu([\pi^a](X))) &= \det\left([\pi^{a_i+1}]_u(X_i)\,\middle|\,[\pi^{a_i}]_u(X_i)^q\,\middle|\,\cdots\,\middle|\,[\pi^{a_i}]_u(X_i)^{q^{h-1}}\right)\\ &=\sum_{\sigma\in S_h}\mathrm{sgn}(\sigma)[\pi^{a_{\sigma(1)}+1}]_u\left(X_{\sigma(1)}\right)\prod_{j=1}^{h-1}[\pi^{a_{\sigma(j+1)}}]_u\left(X_{\sigma(j+1)}\right)^{q^j}\end{aligned}$$

Now assume the X_i are sections of $\mathscr{F}^{\mathrm{univ}}[\pi^n]$: this means that the terms in the sum with $a_{\sigma(1)}=n-1$ vanish. The expression $[\pi]_{\mathrm{LT}}(\mu_n(X_1,\dots,X_n))$ is thus a sum over pairs (a,σ), where $\sigma\in S_h$ is a permutation and $a=(a_1,\dots,a_h)$ is a tuple of integers satisfying the conditions

1. $0\leq a_i\leq n-1$
2. $a_{\sigma(1)}<n-1$
3. $\sum_i a_i=(n-1)(h-1)$

Let $b = (b_1, \dots, b_h)$ be the tuple defined by

$$b_j = \begin{cases} a_j, & j = \sigma(1) \\ a_j - 1, & j \neq \sigma(1) \end{cases}$$

Note that each b_i is nonnegative: If $a_j = 0$ for some $j \neq \sigma(1)$, the condition $\sum_i a_i = (n-1)(h-1)$ forces $a_k = n-1$ for all $k \neq j$, which implies that $a_{\sigma(1)} = n-1$, contradicting condition (ii) above. As (a, σ) runs over all pairs of tuples and permutations satisfying (1)–(3), the pair (b, σ) runs over all pairs of tuples and permutations satisfying $0 \leq b_i \leq n-2$ and $\sum_i b_i = (n-1)(h-1) - (h-1) = (n-2)(h-1)$. We find

$$\begin{aligned} [\pi]_{\mathrm{LT}} \left(\mu_n(X_1, \dots, X_h)\right) &= \sum_{(b,\sigma)} \operatorname{sgn}(\sigma) \prod_{j=1}^{h-1} [\pi^{b_{\sigma(j)+1}}]_u \left(X_{\sigma(j)}\right)^{q^j} \\ &= \sum_b \mu([\pi^{b_1+1}]_u(X_1), \dots, [\pi^{b_h+1}]_u(X_h)) \\ &= \mu_{n-1}\left([\pi]_u(X_1), \dots, [\pi]_u(X_h)\right) \end{aligned}$$

as required. □

Now we can establish the $\mathcal{O}_F$-linearity of μ_n. For this it suffices to show that $\mu_n([\pi]_u(X_1), X_2, \dots, X_{h-1}) = [\pi]_{\mathrm{LT}}(\mu_n(X_1, \dots, X_h))$. We have

$$\mu_n([\pi]_u(X_1), X_2, \dots, X_{h-1}) = \sum_a \mu([\pi^a](X)),$$

where $a = (a_1, \dots, a_{h-1})$ runs over tuples satisfying $1 \leq a_1 \leq n-1$, $0 \leq a_i \leq n-1$ for $i > 1$, and $\sum_i a_i = (h-1)(n-1) + 1$. But these conditions force $a_i \geq 1$ for $i = 1, \dots, h$. Write $a_i = b_i + 1$, so that $0 \leq b_i \leq n-2$ and $\sum_i b_i = (h-1)(n-1)$. Then

$$\begin{aligned} \mu_n([\pi]_u(X_1), X_2, \dots, X_{h-1}) &= \sum_b \mu([\pi^{b_1+1}]_u(X_1), \dots, [\pi^{b_h+1}]_u(X_h)) \\ &= \mu_{n-1}([\pi]_u(X_1), \dots, [\pi]_u(X_h)) \\ &= [\pi]_{\mathrm{LT}}(\mu_n(X_1, \dots, X_h)) \end{aligned}$$

by Prop. 3.7.

We have established part (1) of Thm. 3.2. Part (1) allows us to reduce part (2) to the case of $n = 1$, which has already been treated in Prop. 3.4.

Recall that $X_1^{(n)}, \dots, X_h^{(n)}$ are the canonical coordinates on $\mathfrak{X}(\pi^n)$. Thm. 3.2 shows that the function $\Delta^{(n)} = \mu_n(X_1^{(n)}, \dots, X_h^{(n)})$ is a nonzero root of $[\pi^n]_{\mathrm{LT}}(T)$. The following simple lemma will be useful in the next section.

Lemma 3.8. *Let $M \in M_h(\mathcal{O}_F/\pi^n\mathcal{O}_F)$ be a matrix. Then*

$$\mu_n(M(X_1^{(n)}), \dots, X_h^{(n)}) + \dots + \mu_n(X_1^{(n)}, \dots, M(X_h^{(n)})) = [\operatorname{Tr} M]_{\mathrm{LT}}(\Delta^{(n)}).$$

4 An affinoid with good reduction

We now reach the technical heart of the paper. In this section we will construct an open affinoid neighborhood $\mathfrak{Z}$ around an unramified canonical point x whose reduction is as in Thm. 1.1. These affinoids appear as connected components of the preimage of a subdisc $\mathfrak{X}(1)^1$ inside of the polydisc $\mathfrak{X}(1)$. The polydisc $\mathfrak{X}(1)^1$ is small enough so that the local system $\mathscr{F}^{\mathrm{univ}}[\pi]$ may be trivialized over $\mathfrak{X}(1)^1$, which is to say that the quotient map $\mathfrak{X}(\pi) \to \mathfrak{X}(1)$ admits a section over $\mathfrak{X}(1)^1$. An approximation to this section is computed explicitly in §4.1. A consequence is that the preimage of $\mathfrak{X}(1)^1$ in $\mathfrak{X}(\pi)$ is a disjoint union of polydiscs $\mathfrak{X}(\pi)^{1,x}$ indexed by the canonical points of $\mathfrak{X}(\pi)$.

In §4.2 we turn to the space $\mathfrak{X}(\pi^2)$. An unramified canonical point $x \in \mathfrak{X}(\pi^2)$ determines a subgroup $K_{x,2}$ of $\mathrm{GL}_h(\mathcal{O}_F)$ lying properly between $1+\pi M_h(\mathcal{O}_F)$ and $1+\pi^2 M_h(\mathcal{O}_F)$. Let

$$\mathfrak{X}(K_{x,2}) = \mathfrak{X}(\pi^2)/K_{x,2}.$$

Then the affinoid $\mathfrak{Z}$ of Thm. 1.1 is the preimage of $\mathfrak{X}(\pi)^{1,x}$ in $\mathfrak{X}(K_{x,2})$. We introduce a family of coordinates $Y(\zeta)$ on $\mathfrak{X}(\pi^2)$ which are invariant under $K_{x,2}$, one for each ζ in $\mathcal{O}_E$. (The formation of the $Y(\zeta)$ is modeled on the determinant functor μ_2 from §3.) Thus the $Y(\zeta)$ are analytic functions on $\mathfrak{X}(K_{x,2})$; it turns out (Prop. 4.2) that the $Y(\zeta)$ are integral functions on $\mathfrak{Z}$. A simple linear combination Y of the coordinates $Y(\zeta)$ generates the ring of integral analytic functions on $\mathfrak{Z}$ as an algebra over the ring of integral analytic functions on the polydisc $\mathfrak{X}(\pi)^{x,1}$. The equation for the reduction $\overline{\mathfrak{Z}}$ follows from the congruence calculated in Prop. 4.3.

We often work with affinoid algebras $\mathcal{B}$ over a field E, where E/F is a finitely ramified extension contained in the completion of the separable closure of F. For $f \in \mathcal{B}$ we write $v(f)$ for the infimum of $v(f(z))$ as z runs though $\operatorname{Spm}\mathcal{B}$.

4.1 Analytic sections of $\mathscr{F}^{\mathrm{univ}}[\pi]$

Let E/F be the unramified extension of degree h, so that $\mathcal{O}_E = k_h[\![\pi]\!]$. Let $\mathscr{F}_0$ be the deformation obtained by specializing the variables u_i to 0 in $\mathscr{F}^{\mathrm{univ}}$, so that $[\pi]_{\mathscr{F}_0}(X) = \pi X + X^{q^h}$. Then $\mathscr{F}_0$ admits endomorphisms by $\mathcal{O}_E$. As a formal $\mathcal{O}_E$-module, $\mathscr{F}_0$ has height 1. We will denote by $x^{(0)}$ the unramified canonical point in $\mathfrak{X}(1)$ corresponding to $\mathscr{F}_0$.

For $n \geq 1$, let E_n be the extension of $\hat{E}^{\mathrm{nr}}$ given by adjoining the roots of $[\pi^n]_{\mathscr{F}_0}(X)$. Thus the preimages of $x^{(0)}$ in $\mathfrak{X}(\pi)$ are the points $x = x^{(1)} \in \mathfrak{X}(\pi)$ corresponding to Drinfeld bases $x_1, \dots, x_h \in \mathfrak{p}_{E_1}$ for $\mathscr{F}_0[\pi]$. Let $\mathfrak{X}(1)^1 \subset \mathfrak{X}(1)$ be the affinoid neighborhood defined by the conditions $v(u_i) \geq 1$, $i = 1, \dots, h-1$. Let $V_i = \pi^{-1} u_i$, so that the V_i are a chart of integral coordinates on $\mathfrak{X}(1)^1$. The ring of integral analytic functions on $\mathfrak{X}(1)^1$ is therefore $\hat{\mathcal{O}}_{F^{\mathrm{nr}}}\langle V_1, \dots, V_{h-1}\rangle$. We claim that over $\mathfrak{X}(1)^1 \otimes E_1$, the local system $\mathscr{F}^{\mathrm{univ}}[\pi]$ may be trivialized. This means that every nonzero torsion point of $\mathscr{F}_0[\pi]$ can be "spread out" to a unique section of $\mathscr{F}^{\mathrm{univ}}[\pi]$ over $\mathfrak{X}(1)^1 \otimes E_1$. To be precise:

Proposition 4.1. *The preimage of $\mathfrak{X}(1)^1 \otimes E_1$ in $\mathfrak{X}(\pi)\otimes E_1$ is the disjoint union of polydiscs $\mathfrak{X}(\pi)^{1,x}$ over E_1, each containing a unique unramified canonical point x. For such a point x, corresponding to the basis $x_1,\dots,x_h$ of $\mathscr{F}_0[\pi]$, we have the following congruence, valid in the ring of integral analytic functions on $\mathfrak{X}(\pi)^{1,x}$:*

$$X_r^{(1)} \equiv (-1)^{h-1}\det\begin{pmatrix} V_1 & V_2 & \cdots & V_{h-1} & x_r \\ 1 & V_1^q & \cdots & V_{h-2}^q & x_r^q + \pi x_r V_{h-1}^q \\ 0 & 1 & \cdots & V_{h-3}^{q^2} & x_r^{q^2} + \pi x_r V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & x_r^{q^{h-1}} + \pi x_r V_1^{q^{h-1}} \end{pmatrix} \tag{4.1.1}$$

modulo $\pi^{q-1+\frac{q}{q^h-1}}$.

Proof. Let $x_1,\dots,x_h$ be a basis of $\mathscr{F}_0[\pi]$. Consider the polynomial $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(X) = \pi X + \pi V_1 X^q + \cdots + \pi V_{h-1} X^{q^{h-1}} + X^{q^h} \in \mathcal{O}_F\langle V_1,\dots,V_{h-1}\rangle[X]$. By studying the Newton polygon of the translate $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(X-x_r)$, we find that there is a unique root $X_r \in \mathcal{O}_{E_1}\langle V_1,\dots,V_{h-1}\rangle$ of $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(X)$ for which $v(X_r - x_r) > v(x_r) = 1/(q^h-1)$. This root satisfies $v(X_r - x_r) = v(x_r^q) = q/(q^h-1)$. Then $v(X_r - x_s) = 1/(q^h-1)$ for $r \neq s$. This already implies that the preimage of $\mathfrak{X}(1)^1 \otimes E_1$ in $\mathfrak{X}(\pi)\otimes E_1$ is the union of polydiscs $\mathfrak{X}(\pi)^{1,x}$, where $\mathfrak{X}(\pi)^{1,x}$ is the affinoid described by the inequalities $v(X_r^{(1)} - x_r) \geq v(x_r^q)$, $r = 1,\dots,h$.

Now let $D \in \mathcal{O}_{E_1}[V_1,\dots,V_{h-1}]$ be the expression on the right hand side of Eq. (4.1.1). Expand the determinant in Eq. (4.1.1) along its first row and label the minors $A_1,\dots A_h$, signed appropriately so that

$$D = \sum_{i=1}^{h-1} V_i A_i + x_r A_h. \tag{4.1.2}$$

That is,

$$A_i = (-1)^{h-i}\det\begin{pmatrix} V_1^{q^i} & V_2^{q^i} & \cdots & V_{h-i-1}^{q^i} & x_r^{q^i} + \pi x_r V_{h-i}^{q^i} \\ 1 & V_1^{q^i} & \cdots & V_{h-i-2}^{q^{i+1}} & x_r^{q^{i+1}} + \pi x_r V_{h-i-1}^{q^{i+1}} \\ 0 & 1 & \cdots & V_{h-i-3}^{q^{i+2}} & x_r^{q^{i+2}} + \pi x_r V_{h-i-2}^{q^{i+2}} \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & x_r^{q^{h-1}} + \pi x_r V_1^{q^{h-1}} \end{pmatrix} \tag{4.1.3}$$

for $i = 1,\dots,h-1$, and $A_h = 1$.

In order to complete the proof of Prop. 4.1, we will show that $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(D)$ is sufficiently close to 0 to ensure the congruence in Eq. (4.1.1).

Observe that for $i = 1,\dots,h-1$ we have the following congruence modulo $\pi^{q+\frac{q}{q^h-1}}$:

$$D^{q^i} \equiv (-1)^{h-1} \det \begin{pmatrix} V_1^{q^i} & V_2^{q^i} & \cdots & V_{h-i}^{q^i} & V_{h-i+1}^{q^i} & \cdots & V_{h-1}^{q^i} & x_r^{q^i} \\ 1 & V_1^{q^{i+1}} & \cdots & V_{h-i-1}^{q^{i+1}} & V_{h-i}^{q^{i+1}} & \cdots & V_{h-2}^{q^{i+1}} & x_r^{q^{i+1}} \\ \vdots & & \ddots & \vdots & \vdots & & & \vdots \\ 0 & 0 & \cdots & V_1^{q^{h-1}} & V_2^{q^{h-1}} & \cdots & V_i^{q^{h-1}} & x_r^{q^{h-1}} \\ 0 & 0 & \cdots & 1 & V_1^{q^h} & \cdots & V_{i-1}^{q^h} & -\pi x_r \\ 0 & 0 & \cdots & 0 & 1 & \cdots & V_{i-2}^{q^{h+1}} & 0 \\ \vdots & & & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

Placing the final column of this matrix into position $(h-i+1)$ transforms the above matrix into one of the form $\begin{pmatrix} A & B \\ 0 & C \end{pmatrix}$, where A is a matrix with dimensions $(h-i+1)\times(h-i+1)$ and C is an upper triangular matrix with 1s along the diagonal. We find

$$D^{q^i} \equiv (-1)^{h+i} \det \begin{pmatrix} V_1^{q^i} & V_2^{q^i} & \cdots & V_{h-i-1}^{q^i} & V_{h-i}^{q^i} & x_r^{q^i} \\ 1 & V_1^{q^{i+1}} & \cdots & V_{h-i-2}^{q^{i+1}} & V_{h-i-1}^{q^{i+1}} & x_r^{q^{i+1}} \\ 0 & 1 & \cdots & V_{h-i-3}^{q^{i+2}} & V_{h-i-2}^{q^{i+2}} & x_r^{q^{i+2}} \\ \vdots & & \ddots & & \vdots & \\ 0 & 0 & \cdots & 1 & V_1^{q^{h-1}} & x_r^{q^{h-1}} \\ 0 & 0 & \cdots & 0 & 1 & -\pi x_r \end{pmatrix} \pmod{\pi^{q+\frac{q}{q^h-1}}}. \tag{4.1.4}$$

We can apply elementary row operations to use the 1 in column $h-i$ of this matrix to cancel the entries above it. When this is done, we find

$$D^{q^i} \equiv -A_i \pmod{\pi^{q+\frac{q}{q^h-1}}},\ i=1,\dots,h-1 \tag{4.1.5}$$

where $A_1,\dots,A_{h-1}$ are the minors from Eq. (4.1.3). We also have

$$D^{q^h} \equiv -\pi x_r \equiv -\pi x_r A_h \pmod{\pi^{q+\frac{q}{q^h-1}}}. \tag{4.1.6}$$

Combining Eqs. (4.1.2), (4.1.5) and (4.1.6) gives

$$\begin{aligned} [\pi]_{\mathscr{F}^{\mathrm{univ}}}(D) &= \pi D + \pi V_1 D^q + \cdots + \pi V_{h-1} D^{q^{h-1}} + D^{q^h} \\ &\equiv \pi D - \pi(V_1A_1 + \cdots + V_{h-1}A_{h-1} + x_rA_h) \\ &\equiv 0 \pmod{\pi^{q+\frac{q}{q^h-1}}}. \end{aligned}$$

The ring of integral analytic functions on the polydisc $\mathfrak{X}(\pi)^{1,x}$ is $\mathcal{O}_{E_1}\langle V_1,\dots,V_h\rangle$. In this ring we have the congruences $D \equiv X_r^{(1)} \equiv x_r \pmod{x_r^q}$. Let $Y = D - X_r^{(1)}$. Then $Y \equiv 0 \pmod{x_r^q}$ and $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(Y) \equiv 0 \pmod{\pi^{q+1/(q^h-1)}}$. Examining the Newton polygon of $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(X)$ shows that $Y \equiv 0 \pmod{\pi^{q-1+1/(q^h-1)}}$. □

4.2 Some invariant coordinates on $\mathfrak{X}(\pi^2)$.

Choose a compatible system of bases $x_1^{(n)},\dots,x_h^{(n)}$ for $\mathscr{F}_0[\pi^n]$, $n\geq 1$. This is tantamount to choosing a compatible system of unramified canonical points $x^{(n)}\in\mathfrak{X}(\pi^n)$ lying above the point $x^{(0)}\in\mathfrak{X}(1)$ corresponding to the deformation $\mathscr{F}_0$. Since $\mathscr{F}_0$ admits $\mathcal{O}_F$-linear endomorphisms by $\mathcal{O}_E$, our choice of compatible system induces an embedding of $\mathcal{O}_E$ into $\mathfrak{A}=M_h(\mathcal{O}_F)$, and we identify $\mathcal{O}_E$ with its image. For $M\in\mathfrak{A}$, recall the definition of $M(X_i^{(n)})$ from Eq. (2.3.1). We have $\zeta(X_i^{(n)})(x^{(n)})=\zeta x_i^{(n)}$ for $i=1,\dots,h$, $\zeta\in k_h$.
The unit group $\mathfrak{A}^\times=\mathrm{GL}_h(\mathcal{O}_F)$ has the usual filtration $U_{\mathfrak{A}}^n=1+\mathfrak{p}^n\mathfrak{A}$, $n\geq 1$. Let $C\subset\mathfrak{A}$ be the orthogonal complement of $\mathcal{O}_E$ under the standard trace pairing, and let $\mathfrak{p}_E$ be the maximal ideal of $\mathcal{O}_E$. Define a subgroup $K_{x,2}$ of $\mathfrak{A}^\times$ by

$$K_{x,2}=1+\mathfrak{p}_E^2+\mathfrak{p}_EC,$$

so that $K_{x,2}$ lies between $U_{\mathfrak{A}}^1$ and $U_{\mathfrak{A}}^2$. In what follows we will assume the choice of x is fixed and write simply K_2. Write $\mathfrak{X}(K_2)$ for the quotient of $\mathfrak{X}(\pi^2)$ by K_2.
We shall construct an alternating k-linear expression Y in the canonical coordinates $X_1^{(2)},\dots,X_h^{(2)}$ which is fixed by K_2, so that it descends to an analytic function on $\mathfrak{X}(K_2)$. It happens that Y satisfies a polynomial equation with coefficients in $\mathcal{O}_{E_2}\langle V_1,\dots,V_h\rangle$ whose reduction modulo the maximal ideal of $\mathcal{O}_{E_2}$ gives the smooth hypersurface of Thm. 1.1.
We continue using the shorthand $X_r=X_r^{(1)}$. We introduce the new shorthand $Y_r=X_r^{(2)}$, so that $[\pi]_{\mathscr{F}^{\mathrm{univ}}}(Y_r)=X_r$. Also we let $\Delta=\Delta^{(1)}=\mu(X_1,\dots,X_h)$; this is a locally constant function satisfying $\Delta^{q-1}=(-1)^h\pi$. For $\zeta\in\mathcal{O}_E$, let

$$W(\zeta)=\mu(\zeta(Y_1),X_2,\dots,X_h)+\dots+\mu(X_1,X_2,\dots,\zeta(Y_h)).$$

Note that $W(1)=\mu_2(X_1,\dots,X_h)=\Delta^{(2)}$. We record the action of $U_{\mathfrak{A}}^1$ on the functions $W(\zeta)$: For $g=1+\pi M\in U_{\mathfrak{A}}^1$, we have

$$g(W(\zeta))=W(\zeta)+[\mathrm{Tr}(M\zeta)]_{\mathrm{LT}}(\Delta) \tag{4.2.1}$$

by Lemma 3.8. It follows that $W(\zeta)$ is invariant under K_2, and that $[\pi]_{\mathrm{LT}}(W(\zeta))$ is invariant under $U_{\mathfrak{A}}^1$, so that $[\pi]_{\mathrm{LT}}(W(\zeta))$ belongs to $\mathcal{A}(\pi)$. We can see this directly: by Eq. (3.1.2) we have

$$[\pi]_{\mathrm{LT}}(W(\zeta))=\det\begin{pmatrix}\zeta(X_1) & X_1^q & \cdots & X_1^{q^{h-1}}\\ \vdots & \vdots & \ddots & \vdots\\ \zeta(X_h) & X_h^q & \cdots & X_h^{q^{h-1}}\end{pmatrix}, \tag{4.2.2}$$

which visibly belongs to $\mathcal{A}(\pi)$.
We will use the symbol x to denote our compatible system of canonical points $x^{(n)}\in\mathfrak{X}(\pi^n)$. Then $f(x)$ is well-defined when f is an analytic function on any

of the spaces $\mathfrak{X}(\pi^n)$. We will use $\mathfrak{X}(\pi)^{1,x}$ to refer to the polydisc constructed in §4.1 using the canonical point $x^{(1)}$.
By Prop. 4.1, the restriction of the function $[\pi]_{\mathrm{LT}}(W(\zeta))$ to $\mathfrak{X}(\pi)^{1,x}$ lies in $\mathcal{O}_{E_1}\langle V_1,\dots,V_h\rangle$, where we recall that the variables $V_r = \pi^{-1}u_r$ form our chart of integral coordinates on $\mathfrak{X}(1)^1$. Let $\mathfrak{Z}$ be the preimage of the polydisc $\mathfrak{X}(\pi)^{1,x}$ in $\mathfrak{X}(K_2)\otimes E_2$. It will be useful to transform the functions $W(\zeta)$ into integral functions $Y(\zeta)$ on $\mathfrak{Z}$ for which $|Y(\zeta)|_{\mathfrak{Z}} = 1$. Let $w(\zeta) = W(\zeta)(x)$, and let

$$Y(\zeta) = (-1)^{h-1}\frac{W(\zeta)-w(\zeta)}{\Delta}. \tag{4.2.3}$$

Proposition 4.2. *There exists $\varepsilon > 0$ for which the congruence*

$$Y(\zeta)^q - Y(\zeta) \equiv \begin{pmatrix} V_1 & V_2 & \cdots & V_{h-1} & 0 \\ 1 & V_1^q & \cdots & V_{h-2}^q & (\zeta^q-\zeta)V_{h-1}^q \\ 0 & 1 & \cdots & V_{h-3}^{q^2} & (\zeta^{q^2}-\zeta)V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & (\zeta^{q^{h-1}}-\zeta)V_1^{q^{h-1}} \end{pmatrix} \pmod{\pi^\varepsilon}$$

is valid in the ring of integral analytic functions on $\mathfrak{Z}$.

Proof. The idea is to apply Prop. 4.1 to Eq. (4.2.2). In preparation for this, we need some determinant identities. For $i = 1,\dots,h$, let $B_i \in k[V_1,\dots,V_{h-1}]$ be $(-1)^i$ times the determinant of the top left $i\times i$ submatrix of

$$\begin{pmatrix} V_1 & V_2 & \cdots & V_{h-1} & 0 \\ 1 & V_1^q & \cdots & V_{h-2}^q & V_{h-1}^q \\ 0 & 1 & \cdots & V_{h-3}^{q^2} & V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & V_1^{q^{h-1}} \end{pmatrix}$$

Curiously, the transformation $(V_1,\dots,V_{h-1}) \mapsto (B_1,\dots,B_{h-1})$ is an involution. That is, the determinant of the top left $i\times i$ submatrix of

$$\begin{pmatrix} B_1 & B_2 & \cdots & B_{h-1} & 0 \\ 1 & B_1^q & \cdots & B_{h-2}^q & B_{h-1}^q \\ 0 & 1 & \cdots & B_{h-3}^{q^2} & B_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & B_1^{q^{h-1}} \end{pmatrix}$$

is $(-1)^i V_i$: this can be proven by induction on i. This implies the following identity, valid in the polynomial ring $k[V_1,\dots,V_{h-1},z_1,\dots,z_{h-1}]$:

$$\det\begin{pmatrix} z_1B_1 & z_2B_2 & \cdots & z_{h-1}B_{h-1} & 0 \\ 1 & B_1^q & \cdots & B_{h-2}^q & B_{h-1}^q \\ 0 & 1 & \cdots & B_{h-3}^{q^2} & B_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \ddots & 1 & B_1^{q^{h-1}} \end{pmatrix}$$

$$= \det\begin{pmatrix} V_1 & V_2 & \cdots & V_{h-1} & 0 \\ 1 & V_1^q & \cdots & V_{h-2}^q & z_1V_{h-1}^q \\ 0 & 1 & \cdots & V_{h-3}^{q^2} & z_2V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & z_{h-1}V_1^{q^{h-1}} \end{pmatrix} \quad (4.2.4)$$

This is because both expressions equal

$$z_1B_1V_{h-1}^q + z_2B_2V_{h-2}^{q^2} + \cdots + z_{h-1}B_{h-1}V_1^{q^{h-1}}.$$

According to Prop. 4.1, the coordinate X_r may be expressed modulo $\pi^{q-1+\frac{q}{q^h-1}}$ as a linear combination of the powers $x_r, \dots, x_r^{q^{h-1}}$:

$$X_r \equiv (1-\pi B_h)x_r + B_1x_r^q + B_2x_r^{q^2} + \cdots + B_{h-1}x_r^{q^{h-1}} \pmod{\pi^{q-1+\frac{q}{q^h-1}}}. \quad (4.2.5)$$

For $\zeta \in k_h$ we have

$$\zeta(X_r) \equiv \zeta(1-\pi B_h)x_r + \zeta^q B_1x_r^q + \zeta^{q^2}B_2x_r^{q^2} + \cdots + \zeta^{q^{h-1}}B_{h-1}x_r^{q^{h-1}} \pmod{\pi^{q-1+\frac{q}{q^h-1}}} \quad (4.2.6)$$

Also, for $i = 1, \dots, h-1$ we have

$$X_r^{q^i} \equiv -\pi B_{h-i}^{q^i}x_r + x_r^{q^i} + B_1^{q^i}x_r^{q^{i+1}} + \cdots + B_{h-1-i}^{q^i}x_r^{q^{h-1}} \pmod{\pi^N}, \quad (4.2.7)$$

where $N \geq q + \frac{q}{q^h-1}$. Eqs. (4.2.6) and (4.2.7) may be combined into the congruence of matrices

$$\begin{pmatrix} \zeta(X_1)+E_1 & \cdots & \zeta(X_h)+E_h \\ X_1^q & \cdots & X_h^q \\ \vdots & \ddots & \vdots \\ X_1^{q^{h-1}} & \cdots & X_h^{q^{h-1}} \end{pmatrix}$$
$$\equiv \begin{pmatrix} \zeta(1-\pi B_h) & \zeta^q B_1 & \zeta^{q^2} B_2 & \dots & \zeta^{q^{h-1}} B_{h-1} \\ -\pi B_{h-1}^q & 1 & B_1^q & \cdots & B_{h-2}^q \\ -\pi B_{h-2}^{q^2} & 0 & 1 & \cdots & B_{h-3}^{q^2} \\ \vdots & & & \ddots & \vdots \\ -\pi B_1^{q^{h-1}} & 0 & 0 & \cdots & 1 \end{pmatrix}$$
$$\times \begin{pmatrix} x_1 & \cdots & x_h \\ \vdots & \ddots & \vdots \\ x_1^{q^{h-1}} & \cdots & x_h^{q^{h-1}} \end{pmatrix} \qquad (4.2.8)$$

modulo π^N, where $v(E_i) \geq q-1+q/(q^h-1)$. We take determinants of both sides of Eq. (4.2.8). On the left hand side, we apply Eq. (4.2.2): the determinant is congruent to $[\pi]_{\mathrm{LT}}(W(\zeta))$ modulo an error term π^δ, of valuation

$$\delta \geq q-1+\frac{q}{q^h-1}+\frac{q+q^2+\cdots+q^{h-1}}{q^h-1} = q-1+\frac{q-1}{q^h-1}+\frac{1}{q-1}.$$

On the right hand side, the determinant is Δ times

$$\zeta-\zeta\pi B_h+(-1)^h\pi\det\begin{pmatrix} \zeta^q B_1 & \zeta^{q^2} B_2 & \dots & \zeta^{q^{h-1}} B_{h-1} & 0 \\ 1 & B_1^q & \cdots & B_{h-2}^q & B_{h-1}^q \\ 0 & 1 & \cdots & B_{h-3}^{q^2} & B_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & B_1^{q^{h-1}} \end{pmatrix},$$

and by the identity in Eq. 4.2.4 this equals

$$\zeta+(-1)^h\pi\det\begin{pmatrix} V_1 & V_2 & \dots & V_{h-1} & 0 \\ 1 & V_1^q & \dots & V_{h-2}^q & (\zeta^q-\zeta)V_{h-1}^q \\ 0 & 1 & \dots & V_{h-3}^{q^2} & (\zeta^{q^2}-\zeta)V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & (\zeta^{q^{h-1}}-\zeta)V_1^{q^{h-1}} \end{pmatrix}.$$

Equating determinants of both sides of Eq. (4.2.8) now yields

$$[\pi]_{\mathrm{LT}}(W(\zeta)) \equiv$$

$$\equiv \zeta\Delta + (-1)^h \pi\Delta \det \begin{pmatrix} V_1 & V_2 & \dots & V_{h-1} & 0 \\ 1 & V_1^q & \dots & V_{h-2}^q & (\zeta^q - \zeta)V_{h-1}^q \\ 0 & 1 & \dots & V_{h-3}^{q^2} & (\zeta^{q^2} - \zeta)V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \dots & 1 & (\zeta^{q^{h-1}} - \zeta)V_1^{q^{h-1}} \end{pmatrix} \pmod{\pi^\delta}$$

The functions $V_1, \dots, V_{h-1}$ vanish at the canonical point x; therefore so do the functions $B_1, \dots, B_{h-1}$. Applying the above congruence to x gives

$$[\pi]_{\mathrm{LT}}(w(\zeta)) \equiv \zeta\Delta \pmod{\pi^\delta}. \tag{4.2.9}$$

We have $W(\zeta) = w(\zeta) + (-1)^{h-1}\Delta Y(\zeta)$, so that

$$[\pi]_{\mathrm{LT}}(W(\zeta)) = [\pi]_{\mathrm{LT}}(w(\zeta)) + (-1)^h \pi\Delta(Y(\zeta)^q - Y(\zeta))$$

Therefore the congruence claimed in the proposition is valid modulo π^ε, where

$$\varepsilon = \delta - 1 - \frac{1}{q-1} \geq q - 2 + \frac{q-1}{q^h - 1} > 0.$$

□

The functions $Y(\zeta)$ on $\mathfrak{Z}$ each generate a degree q algebra over the field of meromorphic functions on the polydisc $\mathfrak{X}(\pi)^{1,x}$. But the morphism $\mathfrak{Z} \to \mathfrak{X}(\pi)^{1,x} \otimes E_2$ has degree q^h. We will now construct a linear combination of the $Y(\zeta)$ which generates the entire ring of integral analytic functions on $\mathfrak{Z}$ as an algebra over $\mathcal{O}_{E_2}\langle V_1, \dots, V_{h-1}\rangle$.

Let $\zeta, \zeta^q, \dots, \zeta^{q^h}$ be a basis for k_h/k, and let $\beta \in k_h$ be such that

$$\mathrm{Tr}_{k_h/k}(\beta\zeta^{q^i}) = \begin{cases} 1, & i = 0, \\ 0 & i = 1, \dots, h-1. \end{cases} \tag{4.2.10}$$

This implies that $\beta, \dots, \beta^{q^{h-1}}$ is a basis for k_h/k as well. Let

$$Y = \sum_{i=0}^{h-1} \beta^{q^i} Y(\zeta^{q^i}). \tag{4.2.11}$$

Then the stabilizer of Y in $U_{\mathfrak{A}}^1$ is exactly K_2.

Proposition 4.3. *There exists $\varepsilon > 0$ for which the congruence*

$$Y^{q^h} - Y \equiv \begin{pmatrix} V_1^{q^h} - V_1 & V_2^{q^h} - V_2 & \cdots & V_{h-1}^{q^h} - V_{h-1} & 0 \\ 1 & V_1^q & \cdots & V_{h-2}^q & V_{h-1}^q \\ 0 & 1 & \cdots & V_{h-3}^{q^2} & V_{h-2}^{q^2} \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & V_1^{q^{h-1}} \end{pmatrix} \tag{4.2.12}$$

holds modulo π^ε in the ring of integral analytic functions on $\mathfrak{Z}$.

Proof. We have

$$\begin{aligned}
Y^{q^h}-Y &= \sum_{j=0}^{h-1}\beta^{q^j}\left(Y(\zeta^{q^j})^{q^h}-Y(\zeta^{q^j})\right)\\
&= \sum_{j=0}^{h-1}\beta^{q^j}\sum_{i=0}^{h-1}\left(Y(\zeta^{q^j})^{q}-Y(\zeta^{q^j})\right)^{q^i}\\
&\equiv \sum_{i=0}^{h-1}\sum_{j=0}^{h-1}\beta^{q^j}\det\begin{pmatrix}
V_1^{q^i} & V_2^{q^i} & \cdots & V_{h-1}^{q^i} & 0\\
1 & V_1^{q^{i+1}} & \cdots & V_{h-2}^{q^{i+1}} & (\zeta^{q^{i+j+1}}-\zeta^{q^{i+j}})V_{h-1}^{q^{i+1}}\\
0 & 1 & \cdots & V_{h-3}^{q^{i+2}} & (\zeta^{q^{i+j+2}}-\zeta^{q^{i+j}})V_{h-2}^{q^{i+2}}\\
\vdots & & \ddots & & \vdots\\
0 & 0 & \cdots & 1 & (\zeta^{q^{i+j+h-1}}-\zeta^{q^{i+j}})V_1^{q^{h-1}}
\end{pmatrix}
\end{aligned}$$

modulo π^ε, by Prop. 4.2. We now apply the orthogonality relations in Eq. (4.2.10). The term with $i=0$ is $(-1)^{h-1}B_h$, and the term with $1\le i\le h-1$ is

$$\det\begin{pmatrix}
V_1^{q^i} & V_2^{q^i} & \cdots & V_{h-i}^{q^i} & \cdots & V_{h-1}^{q^i} & 0\\
1 & V_1^{q^{i+1}} & \cdots & V_{h-i-1}^{q^{i+1}} & \cdots & V_{h-2}^{q^{i+1}} & 0\\
0 & 1 & \cdots & V_{h-i-2}^{q^{i+2}} & \cdots & V_{h-3}^{q^{i+2}} & 0\\
\vdots & & & & & & \vdots\\
0 & 0 & \cdots & V_1^{q^{h-1}} & \cdots & V_i^{q^{h-1}} & 0\\
0 & 0 & \cdots & 1 & \cdots & V_{i-1}^{q^h} & V_i^{q^h}\\
0 & 0 & \cdots & 0 & \cdots & V_{i-2}^{q^{h+1}} & 0\\
\vdots & & & \vdots & & & \vdots\\
0 & 0 & \cdots & 0 & \cdots & 1 & 0
\end{pmatrix} = (-1)^{h-1}V_i^{q^h}B_{h-i}^{q^i},$$

so that

$$Y^{q^h}-Y\equiv(-1)^{h-1}(B_h+V_1^{q^h}B_{h-1}+V_2^{q^h}B_{h-2}+\cdots+V_{h-1}^{q^h}B_1)\pmod{\pi^\varepsilon}.$$

This last expression agrees with the determinant in the proposition, as can be seen by expanding along the first row. □

4.3 Conclusion of the proof.

We now complete the proof of Thm. 1.1. Let x be an unramified canonical point on the Lubin-Tate tower. Since the unramified canonical points in $\mathfrak{X}(1)$ lie in the same orbit under $\mathcal{O}_B^\times=\operatorname{Aut}\Sigma$, we may assume that x lies above the point with $u_1=\cdots=u_{h-1}=0$ in $\mathfrak{X}(1)$. Recall that $\mathfrak{X}(\pi)^{1,x}\subset\mathfrak{X}(\pi)\otimes E_1$ is the affinoid defined by the conditions $v(u_i)\ge 1$ for $i=1,\dots,h-1$ and

$v(X_r^{(1)} - x_r) \geq v(x_r^q)$ for $r = 1, \dots, h$; we showed in Prop. 4.1 that $\mathfrak{X}(\pi)^{1,x}$ is a polydisc over E_1.

The quotient $\mathfrak{X}(K_{x,2}) \to \mathfrak{X}(\pi)$ is Galois with group $H = U_{\mathfrak{A}}^1/K_{x,2} \approx \mathbf{F}_{q^h}$. After passing to E_2 coefficients, the affinoid $\mathfrak{Z}$ was defined as the inverse image of $\mathfrak{X}(\pi)^{1,x}$ in this quotient. Therefore $\mathfrak{Z} \to \mathfrak{X}(\pi)^{1,x} \otimes E_2$ is an étale cover of affinoids with group H. Consider the integral coordinate Y on $\mathfrak{Z}$ produced by Prop. 4.3: the calculation in §5.1 below shows that the action of a nonzero element of H translates Y by a nonzero element of $\mathbf{F}_{q^h}$. Thus the reduction of the cover $\mathfrak{Z} \to \mathfrak{X}(\pi)^{1,x} \otimes E_2$ is an étale cover of affine hypersurfaces over $\overline{k}$, also with group H.

For a tuple $V = (V_1, \dots, V_{h-1})$, let $d(V)$ denote the determinant appearing on the right hand side of Eq. (4.2.12). Let $\overline{\mathfrak{Z}}'$ denote the hypersurface over $\overline{k}$ with equation $Y^{q^h} - Y = d(V)$; then $\overline{\mathfrak{Z}}' \to \mathbf{A}^{h-1}$ is an Artin-Schreier cover of affine hypersurfaces with group H. Prop. 4.3 shows that $\overline{\mathfrak{Z}} \to \mathbf{A}^{h-1}$ factors through an H-equivariant morphism $\overline{\mathfrak{Z}} \to \overline{\mathfrak{Z}}'$. Since $\overline{\mathfrak{Z}}$ and $\overline{\mathfrak{Z}}'$ are both étale covers of $\mathbf{A}^{h-1}$ with group H, we find that $\overline{\mathfrak{Z}} \to \overline{\mathfrak{Z}}'$ is an isomorphism.

Finally, $\overline{\mathfrak{Z}}'$ is isomorphic to the hypersurface described in Thm. 1.1 via $Y = (-1)^{h-1}V_h$. This concludes the proof of Thm. 1.1.

5 Group actions on a hypersurface

We close with a discussion of various group actions on the affinoid $\mathfrak{Z}$, with an eye towards linking Thm. 1.1 with the local Langlands correspondence and the Jacquet-Langlands correspondence. What follows is meant to indicate further directions of research; no proofs will be given.

A large open subgroup of $\mathrm{GL}_h(F) \times B^\times \times W_F$ acts on the Lubin-Tate tower $\mathfrak{X}(\pi^n)$, cf. the introduction to [HT01]. To investigate the question of whether the cohomology of the affinoid $\mathfrak{Z}$ realizes the appropriate correspondences among the three factor groups, it will be useful to compute the stabilizer of $\mathfrak{Z}$ in each group, along with the action of the stabilizer on the reduction $\overline{\mathfrak{Z}}$. We do precisely this for the groups $\mathrm{GL}_h(F)$ and W_F. The hypersurface $\overline{\mathfrak{Z}}$, when considered as an abstract variety over $\overline{k}$, admits a nontrivial action by a large subquotient of $B^\times$, but we cannot prove this action arises from the actual action of $B^\times$ on the Lubin-Tate tower.

Let X be the $\mathbf{F}_{q^h}$-rational model for $\overline{\mathfrak{Z}}/\overline{\mathbf{F}}_q$ from Conj. 1.6. That is, $X \subset \mathbf{A}^h_{\mathbf{F}_{q^h}}$ is the hypersurface with equation

$$\det \begin{pmatrix} V_1^{q^h} - V_1 & V_2^{q^h} - V_2 & V_3^{q^h} - V_3 & \cdots & V_{h-1}^{q^h} - V_{h-1} & V_h^{q^h} - V_h \\ 1 & V_1^q & V_2^q & \cdots & V_{h-2}^q & V_{h-1}^q \\ 0 & 1 & V_1^{q^2} & \cdots & V_{h-3}^{q^2} & V_{h-2}^{q^2} \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 & V_1^{q^{h-1}} \end{pmatrix} = 0.$$

The actions on $\overline{\mathfrak{Z}}$ we consider in this paragraph all descend to actions on the $\mathbf{F}_{q^h}$-rational model X.

5.1 The action of $\mathrm{GL}_h(F)$

The affioid $\mathfrak{Z}$ is stabilized by the group $U^1_{\mathfrak{A}} = 1 + \pi M_h(\mathcal{O}_F)$, and the action of $U^1_{\mathfrak{A}}$ on $\mathfrak{Z}$ factors through the quotient $H = U^1_{\mathfrak{A}}/K_2$. The action of H on the reduction $\overline{\mathfrak{Z}}$ can be made completely explicit. We identify H with $k_h = \mathbf{F}_{q^h}$ via the isomorphism $1+\gamma\pi \mapsto \gamma$, $\gamma \in k_h$. From Eq. (4.2.1) and the construction of Y in Eqs. (4.2.3) and (4.2.11) we see that the action of an element $\gamma \in H$ on $\overline{\mathfrak{Z}}$ preserves the variables $V_1, \dots, V_{h-1}$ and has the following effect on V_h:

$$V_h \mapsto V_h + \sum_{j=1}^{h-1} \beta^{q^j} \operatorname{Tr}_{k_h/k}(\zeta^{q^j}\gamma) = V_h + \gamma. \tag{5.1.1}$$

Of course, this action descends to an action of H on X by $\mathbf{F}_{q^h}$-rational automorphisms.

We offer some brief remarks relating the characters of the group H to the theory of Bushnell-Kutzko types for $\mathrm{GL}_h(F)$, wherein supercuspidal representations are constructed by induction from compact-mod-center subgroups. In fact, in our particular situation, the construction goes back to Howe [How77]. Suppose ψ is a character of $H \approx \mathbf{F}_{q^h}$ which does not factor through $\operatorname{Tr}_{\mathbf{F}_{q^h}/\mathbf{F}_{q^d}}$ for any proper divisor d of h. This character pulls back to a character of $U^1_{\mathfrak{A}} = 1+\pi M_h(\mathcal{O}_F)$, which we also call ψ. Recall that we have fixed an embedding of E into $M_h(F)$. Choose a character θ of $E^\times$ for which $\theta|_{1+\mathfrak{p}_E} = \psi|_{1+\mathfrak{p}_E}$. Then θ is an *admissible* character in the sense that there is no proper subextension $E' \subset E$ of E/F for which θ factors through the norm map $E^\times \to (E')^\times$. The character θ has conductor $\mathfrak{p}_E^2$. Let η be the unique character of $J = E^\times U^1_{\mathfrak{A}}$ for which $\eta|_{E^\times} = \theta$ and $\eta|_{U^1_{\mathfrak{A}}} = \psi$. Then $\pi(\theta) = \operatorname{Ind}_J^{\mathrm{GL}_h(F)} \eta$ is a supercuspidal representation of $\mathrm{GL}_h(F)$ of level π^2: This is a special case of the construction used to prove Theorem 2 of [How77].

Therefore the question of whether the cohomology of $\mathfrak{Z}$ realizes the Bushnell-Kutzko types for $\mathrm{GL}_h(F)$ is a matter of determining which characters of H appear in the cohomology of X; this is discussed in Conj. 5.1 below.

5.2 The action of inertia

The action of the inertia subgroup $I_F \subset W_F$ on $\overline{\mathfrak{Z}}$ can be made explicit as well. Let $I_2 = \mathrm{Gal}(E_2/E^{\mathrm{nr}})$; we identify I_2 with $(\mathcal{O}_E/\pi^2\mathcal{O}_E)^\times$ via the reciprocity map of local class field theory. Thus if $\alpha \in \mathcal{O}_E^\times$, and $x \in \mathfrak{X}(\pi^2)$ is an unramified canonical point corresponding to a basis $x_1, \dots, x_h$ of $\mathscr{F}_0[\pi^2]$, then $\alpha(x)$ corresponds to the basis $\alpha x_1, \dots, \alpha x_h$. Since the definition of the affinoid $\mathfrak{Z}$ only depends on the image of x in $\mathfrak{X}(\pi)$, the stabilizer of $\mathfrak{Z}$ in I_2 is the group $(1+\pi\mathcal{O}_E)/(1+\pi^2\mathcal{O}_E)$. The action of an element $1+\gamma\pi \in 1+\pi\mathcal{O}_E$ on $\overline{\mathfrak{Z}}$ is exactly as in Eq. (5.1.1).

5.3 The action of $B^\times$

More subtle is the action of $\mathcal{O}_B^\times = \operatorname{Aut}\Sigma$. The algebra $\mathcal{O}_B$ is generated over $\mathcal{O}_F$ by $\mathcal{O}_E$ and Φ, where $\Phi^h = \pi$ and $\Phi\alpha = \alpha^q\Phi$, $\alpha \in \mathcal{O}_E$. For $n \geq 1$, let $U_B^n = 1 + \Phi^n\mathcal{O}_B$. Let C^B be the orthogonal complement of $\mathcal{O}_E$ in $\mathcal{O}_B$, so that

$$C^B = \mathcal{O}_E\Phi \oplus \cdots \oplus \mathcal{O}_E\Phi^{h-1},$$

and define a subgroup K_2^B of $\mathcal{O}_B^\times$ by

$$K_2^B = 1 + \mathfrak{p}_E^2 + \mathfrak{p}_E C,$$

so that K_2^B lies properly between U_B^1 and U_B^2. Let $H^B = U_B^1/K_2^B$. Let R be the noncommutative ring $\mathbf{F}_{q^h}[\tau]/(\tau^{h+1})$ whose multiplication is given by the rule $\alpha\tau = \tau\alpha^q$, $\alpha \in \mathbf{F}_{q^h}$. Then H^B is isomorphic to $1 + \tau R$. As we observed in Rmk. 1.2, $R^\times$ acts on X. It seems likely that the stabilizer of $\mathfrak{Z}$ in $\mathcal{O}_B^\times$ is U_B^1, and that the action of U_B^1 on $\overline{\mathfrak{Z}}$ factors through the this action of $H^B \cong 1+\tau R$. The action of such a large group of $\mathbf{F}_{q^h}$-rational automorphisms has consequences for the cohomology of X which allow us to reinterpret Conj. 1.6. First, let us provide a short description of the representation theory of the nilpotent group H^B. The subgroup $Z = 1 + \tau^h R$ is the center of $1 + \tau R \cong H^B$. Let ψ be a character of $Z \approx \mathbf{F}_{q^h}$ which does not factor through $\operatorname{Tr}_{\mathbf{F}_{q^h}/\mathbf{F}_{q^d}}$ for any proper divisor d of h. There is a unique representation V_ψ of H^B lying over ψ, of dimension $q^{h(h-1)/2}$. Let $\mathcal{H} = H_c^*(X \otimes \overline{\mathbf{F}}_q, \overline{\mathbf{Q}}_\ell)$, considered as a virtual module for the action of $\operatorname{Gal}(\overline{\mathbf{F}}_q/\mathbf{F}_{q^h}) \times H^B$. Conj. 1.6 now takes the following alternate form:

Conjecture 5.1. *Let $\mathcal{H}_\psi = \operatorname{Hom}_{H^B}(V_\psi, \mathcal{H})$, considered as a virtual module for the action of $\operatorname{Gal}(\overline{\mathbf{F}}_q/\mathbf{F}_{q^h})$. Then $\dim \mathcal{H}_\psi = (-1)^{h-1}$, and the eigenvalue of $\operatorname{Frob}_{q^h}$ on $\mathcal{H}_\psi$ is $q^{h(h-1)/2}$.*

The formalism of Bushnell-Kutzko types for $\mathrm{GL}_h(F)$ in [BK93] has been extended to the context of its anisotropic form $B^\times$ by Broussous [Bro95]. Granting Conj. 5.1, it will not be difficult to detect the types for $B^\times$ in the middle cohomology of $\mathfrak{Z}$. The types for $B^\times$ appearing in $H_c^{h-1}(\overline{\mathfrak{Z}}, \overline{\mathbf{Q}}_\ell)$ should correspond exactly to those types for $\mathrm{GL}_h(F)$ which appear there; indeed this space should realize the correspondence between types. There has already been much work towards an "explicit Jacquet-Langlands correspondence", whereby the admissible square-integrable duals of $\mathrm{GL}_h(F)$ and of $B^\times$ are linked via the explicit parameterizations of each dual via types, see [Hen93], [BH00], [BH05c]. However there are still outstanding cases where the explicit Jacquet-Langlands correspondence is not established, including (in some instances) the supercuspidals $\pi(\theta)$ of §5.1. For these there may be some advantage to the cohomological point of view, given that the Jacquet-Langlands correspondence is already known to be realized in the cohomology of the Lubin-Tate tower, cf. [HT01], [Str08a].

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Dimensions of Affine Deligne-Lusztig Varieties in Affine Flag Varieties

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Abstract. Affine Deligne-Lusztig varieties are analogs of Deligne-Lusztig varieties in the context of an affine root system. We prove a conjecture stated in the paper [5] by Haines, Kottwitz, Reuman, and the first named author, about the question which affine Deligne-Lusztig varieties (for a split group and a basic σ-conjugacy class) in the Iwahori case are non-empty. If the underlying algebraic group is a classical group and the chosen basic σ-conjugacy class is the class of $b = 1$, we also prove the dimension formula predicted in op. cit. in almost all cases.

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1 Introduction

1.1

Affine Deligne-Lusztig varieties, which are analogs of usual Deligne-Lusztig varieties [3] in the context of an affine root system, have been studied by several people, mainly because they encode interesting information about the reduction of Shimura varieties and specifically about the relation between the "Newton stratification" and the "Kottwitz-Rapoport stratification". Their definition is purely group-theoretical. To recall it, we fix a split connected reductive group over the finite field $\mathbb{F}_q$ with q elements. Let $\Bbbk$ be an algebraic closure of $\mathbb{F}_q$, let $L = \Bbbk((\epsilon))$ be the field of formal Laurent series over $\Bbbk$, and let σ be the

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automorphism of L defined by $\sigma(\sum a_n\epsilon^n) = \sum a_n^q \epsilon^n$. We also denote the induced automorphism on the loop group $G(L)$ by σ. Let $T \subset G$ be a split maximal torus, and denote by W the corresponding Weyl group. Furthermore, let $I \subset G(\Bbbk[[\epsilon]])$ be an Iwahori subgroup containing $T(\Bbbk[[\epsilon]])$, and let $\tilde{W}$ be the extended affine Weyl group attached to these data. See Section 2.1 for details. For $x \in \tilde{W}$ and $b \in G(L)$ the locally closed subscheme

$$X_x(b) = \{g \in G(L)/I;\ g^{-1}b\sigma(g) \in IxI\}$$

of the affine flag variety $G(L)/I$ is called the *affine Deligne-Lusztig variety* attached to b and x. The $X_x(b)$ are known to be finite-dimensional varieties (locally of finite type over $\Bbbk$), but are possibly empty, and it is not in general easy to check whether $X_x(b) = \emptyset$ for a given pair x, b.
In [5, Conjecture 9.5.1 (a)] , Haines, Kottwitz, Reuman and the first named author have stated the following conjecture, which extends a conjecture formulated earlier by Reuman. For simplicity, let us assume that G is quasi-simple of adjoint type.
We denote by $\tilde{W}'$ the lowest two-sided cell in the sense of Kazhdan and Lusztig. In the terminology of [5], this is the union of the shrunken Weyl chambers. See Section 2.3. The notion of *basic* σ-conjugacy class can be characterized by saying that it contains an element of $N(T)(L)$ which gives rise to a length 0 element of $\tilde{W} = N(T)(L)/T(\Bbbk[[\epsilon]])$. Equivalently, a σ-conjugacy class is basic if and only if its Newton vector is central. See [5, Lemma 7.2.1]. The σ-conjugacy class of $b = 1$ is always basic.

Conjecture 1.1.1. *Suppose that the σ-conjugacy class of b is basic, and that $x \in \tilde{W}'$. If b and x are in the same connected component of $G(L)$ and*

$$\eta(x) \in W \setminus \bigcup_{T \subsetneq S} W_T,$$

then $X_x(b) \neq \emptyset$ and

$$\dim X_x(b) = \frac{1}{2}\left(\ell(x) + \ell(\eta(x)) - \operatorname{def}_G(b)\right).$$

Here S is the set of simple reflections, and for any $T \subset S$, W_T denotes the subgroup of W generated by T. Furthermore, η is the map $\tilde{W} \to W$ given as follows: If $x = vt^\mu w$ with $v, w \in W$ and such that the alcove $t^\mu w$ lies in the dominant chamber, then $\eta(x) = wv$. See Section 3.1. Finally, $\operatorname{def}_G(b)$ is the defect of b, see [11].
A strengthened version of the converse of the non-emptiness statement was proved in [5, Proposition 9.5.4]. Here we prove

Theorem 1.1.2. *Suppose that the σ-conjugacy class of b is basic, and that $x \in \tilde{W}'$. Write $x = vt^\mu w$ as above. Assume that b and x are in the same connected component of $G(L)$ and that*

$$\eta(x) \in W \setminus \bigcup_{T \subsetneq S} W_T.$$

1. *Then* $X_x(b) \neq \emptyset$.

2. *If* v *equals* w_0*, the longest element of* W*, or* μ *is regular, then*

$$\dim X_x(b) \leqslant \frac{1}{2}\left(\ell(x) + \ell(\eta(x)) - \mathrm{def}_G(b)\right).$$

3. *If* G *is a classical group and* $b = 1$*, or of type* A_n *and* b *arbitrary basic, then*

$$\dim X_x(b) \geqslant \frac{1}{2}\left(\ell(x) + \ell(\eta(x)) - \mathrm{def}_G(b)\right).$$

See Section 3.1 for more detailed statements and an outline of the proof. Roughly speaking, our methods are combinatorial (whereas in [5] the theory of ϵ-adic groups was used). Important ingredients are a refinement of the reduction method of Deligne and Lusztig (Section 2), and the results of the second named author about conjugacy classes in affine Weyl groups, see [9].
In [1], E. Beazley obtained similar results for groups of type A_n, C_2 or G_2 using a similar method, but using only results on conjugacy classes in finite Weyl groups.
In Section 4, we briefly consider the case that $x \in \tilde{W} \setminus \tilde{W}'$, but all in all this case remains unclear. Note however that the relation to stratifications of the wonderful compactification of G might provide further insight in this case, see [10]. Finally, a careful study of the reduction method also shows that affine Deligne-Lusztig varieties in the affine flag varieties are not equidimensional in general; we give a specific example in Section 5. Note that for affine Deligne-Lusztig varieties in the affine Grassmannian, equidimensionality is known. For b in the torus $T(L)$, this was proved in [4, Proposition 2.17.1], and for basic b in [6, Theorem 1.2]; for the intermediate cases, see [7, Corollary 6.8 (a)].

2 Preliminaries

2.1 Notation

Let G be a split connected reductive group over $\mathbb{F}_q$. We assume that G is quasi-simple of adjoint type. As explained in [4, 5.9], all problems about the dimension of affine Deligne-Lusztig varieties easily reduce to this case.
Let $L = \Bbbk((\epsilon))$ be the field of formal Laurent series over $\Bbbk$, and let σ be the automorphism on L defined by $\sigma(\sum a_n \epsilon^n) = \sum a_n^q \epsilon^n$. We also denote the induced automorphism on the loop group $G(L)$ by σ.
Let T be a maximal torus of G, let $B \supset T$ be a Borel subgroup of G, and let B^- be the opposite Borel subgroup so that $T = B \cap B^-$. Let Φ be the set of roots and Y be the coweight lattice. We denote by Y_+ the set of dominant coweights. Let $(\alpha_i)_{i \in S}$ be the set of simple roots determined by (B, T). We denote by W the Weyl group $N(T)/T$. For $i \in S$, we denote by s_i the simple reflection corresponding to i.

For $w \in W$, we denote by $\mathrm{supp}(w)$ the set of simple reflections occurring in a reduced expression of w. So the condition $w \in W \setminus \bigcup_{T \subsetneq S} W_T$ is equivalent to $\mathrm{supp}(w) = S$.

For $w \in W$, we choose a representative in $N(T)$ and also write it as w. For any $J \subset S$, let Φ_J^+ (resp. Φ_J^-) be the positive (resp. negative) roots spanned by $(\alpha_j)_{j \in J}$.

Let I be the inverse image of B^- under the projection map $G(\Bbbk[[\epsilon]]) \to G$ sending ϵ to 0. Let $\tilde{W} = N(T(L))/(T(L) \cap I)$ be the extended affine Weyl group of $G(L)$. Then it is known that $\tilde{W} = W \ltimes Y = \{w\epsilon^\chi; w \in W, \chi \in Y\}$. Let $\ell : \tilde{W} \to \mathbb{N} \cup \{0\}$ be the length function. For $x = w\epsilon^\chi \in \tilde{W}$, we also write x for the representative $w\epsilon^\chi$ in $N(T(L))$.

Let X be the coroot lattice, and let $W_a = W \ltimes X \subset \tilde{W}$ be the affine Weyl group. Set $\tilde{S} = S \cup \{0\}$ and $s_0 = \epsilon^{\theta^\vee} s_\theta$, where θ is the largest positive root of G. Then $(W_a, \tilde{S})$ is a Coxeter system. Let $\kappa : \tilde{W} \to \tilde{W}/W_a$ be the natural projection.

For any $J \subset \tilde{S}$, let W_J be the subgroup of W_a generated by J and $\tilde{W}^J$ (resp. ${}^J\tilde{W}$) be the set of minimal length coset representative of $\tilde{W}/W_J$ (resp. $W_J \backslash \tilde{W}$). For example, ${}^S\tilde{W}$ is the set of all elements for which the corresponding alcove is contained in the dominant chamber. In the case where $J \subset S$, we write W^J for $\tilde{W}^J \cap W$ and ${}^J W$ for ${}^J\tilde{W} \cap W$.

Let λ be a dominant coweight. Set $I(\lambda) = \{i \in S; \langle \lambda, \alpha_i \rangle = 0\}$, the "set of walls" that λ lies on. For $J \subset S$, let $\rho_J^\vee \in Y_+$ with

$$\langle \rho_J^\vee, \alpha_i \rangle = \begin{cases} 1, & \text{if } j \in J \\ 0, & \text{if } j \notin J \end{cases}.$$

We simply write $\rho^\vee$ for $\rho_S^\vee$.

For any root $\alpha \in \Phi$, set $\delta_\alpha = \begin{cases} 1, & \text{if } \alpha \in \Phi^- \\ 0, & \text{if } \alpha \in \Phi^+ \end{cases}$.

2.2

Following [9, 1.4], we use the following notation: For $x, x' \in \tilde{W}$ and $i \in \tilde{S}$, we write $x \xrightarrow{s_i} x'$ if $x' = s_i x s_i$ and $\ell(x') \leqslant \ell(x)$. We write $x \tilde{\to} x'$ if there is a sequence $x = x_0, x_1, \cdots, x_n = x'$ of elements in $\tilde{W}$ such that for all k, $x_k = \tau x_{k-1} \tau^{-1}$ for some $\tau \in \tilde{W}$ with $\ell(\tau) = 0$ or $x_{k-1} \xrightarrow{s_i} x_k$ for some $i \in \tilde{S}$. We write $x \tilde{\approx} x'$ if $x \tilde{\to} x'$ and $x' \tilde{\to} x$.

2.3

Any element in $\tilde{W}$ can be written in a unique way as $vt^\mu w$ for $\mu \in Y_+$, $v \in W$ and $w \in {}^{I(\mu)}W$. Note that in this case $t^\mu w \in {}^S\tilde{W}$, and $\ell(v\tau^\mu w) = \ell(v) + \ell(t^\mu) - \ell(w)$. Set

$$\tilde{W}' = \{vt^\mu w;\ \mu \in Y_+,\ w \in {}^{I(\mu)}W,\ \langle \mu, \alpha_i \rangle + \delta_{v\alpha_i} - \delta_{w^{-1}\alpha_i} \neq 0 \quad \forall i \in S\}.$$

It is proved by Lusztig [12], Shi [13] and Bédard [2] that $\tilde{W}' \cap C$ is a two-sided cell for each W_a-coset C in $\tilde{W}$. It is called the *lowest two-sided cell.* It is also called the union of the *shrunken Weyl chambers* in [4] and [5].

2.4

We introduce a convenient notation for varieties of tuples of elements in Flag $=$ $G(L)/I$ (i.e., the affine flag variety of G over $\Bbbk$). Instead of giving a rigorous definition, it is more useful to explain the notation by examples. We denote by $\mathcal{O}_w \subset \mathrm{Flag} \times \mathrm{Flag}$ the locally closed subvariety of pairs (g, g') such that the relative position of g and g' is w. Then we set

$$\{\, g \xrightarrow{w} g'' \xrightarrow{w'} g' \,\} :=$$
$$\{(g, g', g'') \in (\mathrm{Flag})^3;\ (g, g'') \in \mathcal{O}_w,\ (g'', g') \in \mathcal{O}_{w'}\}.$$

Similarly,

$$\{\, \underbrace{g \xrightarrow{w} g'' \xrightarrow{w'} g'}_{w''} \,\} :=$$
$$\{(g, g', g'') \in (\mathrm{Flag})^3;\ (g, g'') \in \mathcal{O}_w,\ (g'', g') \in \mathcal{O}_{w'},\ (g, g') \in \mathcal{O}_{w''}\}.$$

Finally, we need conditions on relative positions where elements g and $b\sigma(g)$ occur both—the simplest case being the affine Deligne-Lusztig varieties themselves:

$$X_x(b) = \{\, g \xrightarrow{x} b\sigma(g) \,\}.$$

In all these cases, we do not distinguish between the sets given by the conditions on the relative position, and the corresponding locally closed sub-ind-schemes of the product of affine flag varieties.

The following properties are easy to prove.

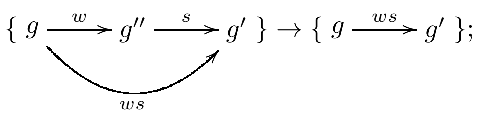
(1) Let $x, y \in \tilde{W}$. If $l(xy) = l(x) + l(y)$, then the map $(g, g', g'') \mapsto (g, g')$ gives an isomorphism

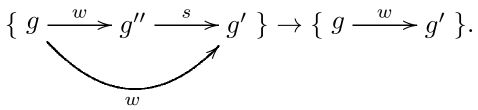
$$\{\, \underbrace{g \xrightarrow{x} g'' \xrightarrow{y} g'}_{xy} \,\} \to \{\, g \xrightarrow{xy} g' \,\}.$$

(2) Let $w \in \tilde{W}$ and $s \in \tilde{S}$. If $ws < w$, then

$$\{\, g \xrightarrow{w} g'' \xrightarrow{s} g' \,\} = \{\, \underbrace{g \xrightarrow{w} g'' \xrightarrow{s} g'}_{ws} \,\} \sqcup \{\, \underbrace{g \xrightarrow{w} g'' \xrightarrow{s} g'}_{w} \,\},$$

where the first set on the right hand side of the equation is open, and the second one is closed. The projections $(g, g', g'') \mapsto (g, g')$ give rise to Zariski-locally trivial fiber bundles





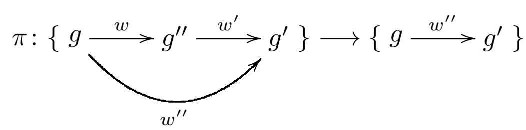
with fibers isomorphic to $\mathbb{A}^1$ in the first case, and isomorphic to $\mathbb{A}^1 \setminus \{0\}$ in the second case.

2.5 The reduction method of Deligne and Lusztig

Lemma 2.5.1 (He [8], Lemma 1). *Let $w, w' \in \tilde{W}$. Then the set $\{uu';\ u \leqslant w,\ u' \leqslant w'\}$ has a unique maximal element, which we denote by $w * w'$. We have $\ell(w * w') = \ell(w) + \ell(w^{-1}(w * w')) = \ell((w * w')(w')^{-1}) + \ell(w')$, and $\operatorname{supp}(w * w') = \operatorname{supp}(w) \cup \operatorname{supp}(w')$.*

Note that the operation $*$ is associative.

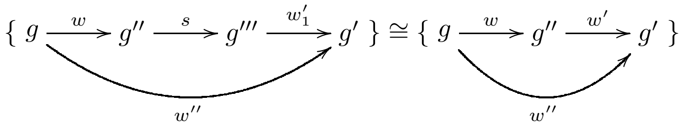
Proposition 2.5.2. *Let $w, w' \in \tilde{W}$, and let $w'' \in \{ww', w * w'\}$. All fibers of the projection*



which maps (g, g', g'') to (g, g') have dimension

$$\dim \pi^{-1}((g, g')) \geqslant \begin{cases} \ell(w) + \ell(w') - \ell(w * w') & \text{if } w'' = w * w', \\ \frac{1}{2}(\ell(w) + \ell(w') - \ell(ww')) & \text{if } w'' = ww'. \end{cases}$$

Proof. We proceed by induction on $\ell(w')$. If $w' = 1$, then the statement is obvious. Now assume that $l(w') > 0$. Then $w' = sw'_1$ for some $s \in \tilde{S}$ and $w'_1 \in \tilde{W}$ with $\ell(w') = \ell(w'_1) + 1$. Then



If $ws > w$, then

$$\{ g \xrightarrow{w} g'' \xrightarrow{s} g''' \xrightarrow{w_1'} g' \ (g \xrightarrow{w''} g') \} \cong \{ g \xrightarrow{ws} g''' \xrightarrow{w_1'} g' \ (g \xrightarrow{w''} g') .\}$$

We also have that $\ell(ws) + \ell(w_1') = \ell(w) + 1 + \ell(w') - 1 = \ell(w) + \ell(w')$, $wsw_1' = ww'$ and $(ws) * w_1' = w * s * w_1' = w * w'$. Now the statement follows from inductive hypothesis on w_1'.
If $ws < w$, then

$$\{ g \xrightarrow{w} g'' \xrightarrow{s} g''' \xrightarrow{w_1'} g' \ (g \xrightarrow{w''} g') \} = X_1 \sqcup X_2,$$

where

$$X_1 = \{ g \xrightarrow{w} g'' \xrightarrow{s} g''' \xrightarrow{w_1'} g' \ (g \xrightarrow{ws} g''',\ g \xrightarrow{w''} g') \}$$

$$X_2 = \{ g \xrightarrow{w} g'' \xrightarrow{s} g''' \xrightarrow{w_1'} g' \ (g \xrightarrow{w} g''',\ g \xrightarrow{w''} g') \}.$$

The projection from X_1 to $\{ g \xrightarrow{w''} g' \}$ factors through

$$X_1 \to \{ g \xrightarrow{ws} g''' \xrightarrow{w_1'} g' \ (g \xrightarrow{w''} g') \} \to \{ g \xrightarrow{w''} g' \},$$

where the first map is a bundle map whose fibers are all of dimension 1. If $w'' = ww'$, then by induction hypothesis on w_1', the fibers of the second map all have dimension $\geqslant \frac{1}{2}(\ell(ws) + \ell(w_1') - l(ww'))$. Notice that $\ell(ws) + \ell(w_1') = \ell(w) - 1 + \ell(w') - 1 = \ell(w) + \ell(w') - 2$. So the fibers of the map $X_1 \to \{ g \xrightarrow{w''} g' \}$ all have dimension $\geqslant \frac{1}{2}(\ell(w) + \ell(w') - l(ww'))$, which gives us the desired lower bound on the fiber dimension.

The projection from X_2 to $\{\ g \xrightarrow{w''} g'\ \}$ factors through

$$X_2 \to \{\ g \xrightarrow{w} g''' \xrightarrow{w_1'} g',\ g \xrightarrow{w''} g'\ \} \to \{\ g \xrightarrow{w''} g'\ \},$$

where the first map is a bundle map whose fibers are all of dimension 1. If $w'' = w{*}w' = w{*}s{*}w_1' = w{*}w_1'$, then by induction hypothesis on w_1', the fibers of the second map all have dimension $\geqslant (\ell(w) + \ell(w_1') - \ell(w * w'))$. Notice that $\ell(w) + \ell(w_1') = \ell(w) + \ell(w') - 1$. So the fibers of the map $X_2 \to \{\ g \xrightarrow{w''} g'\ \}$ all have dimension $\geqslant (\ell(w) + \ell(w') - \ell(w * (w'))$. □

As a corollary, we can prove the analog, in the affine context, of the "reduction method" of Deligne and Lusztig (see [3, proof of Theorem 1.6]). This result can of course be proved directly, along the lines of the proof of the proposition above, and was also worked out before by Haines at the suggestion of Lusztig.

Corollary 2.5.3. *Let $x \in \widetilde{W}$, and let $s \in \tilde{S}$ be a simple affine reflection.*

1. *If $\ell(sxs) = \ell(x)$, then there exists a universal homeomorphism $X_x(b) \to X_{sxs}(b)$.*
2. *If $\ell(sxs) = \ell(x) - 2$, then $X_x(b)$ can be written as a disjoint union $X_x(b) = X_1 \sqcup X_2$ where X_1 is closed and X_2 is open, and such that there exist morphisms $X_1 \to X_{sxs}(b)$ and $X_2 \to X_{sx}(b)$ which are compositions of a Zariski-locally trivial fiber bundle with one-dimensional fibers and a universal homeomorphism.*

Proof. By possibly exchanging, in case (1), x and sxs, we may assume that $sx < x$. By the proposition, the projection

$$X' := \left\{ \begin{array}{ccc} g & \xrightarrow{x} & b\sigma(g) \\ {\scriptstyle s}\downarrow & \overset{sx}{\nearrow} & \downarrow{\scriptstyle s} \\ g_1 & & b\sigma(g_1) \end{array} \right\} \longrightarrow \{\ g \xrightarrow{x} b\sigma(g)\ \} = X_x(b).$$

is an isomorphism, so we may replace $X_x(b)$ by X'. We write X' as the disjoint union

$$X' = X_1 \sqcup X_2 := \left\{ \begin{array}{ccc} g & \xrightarrow{x} & b\sigma(g) \\ {\scriptstyle s}\downarrow & \overset{sx}{\nearrow} & \downarrow{\scriptstyle s} \\ g_1 & \xrightarrow[sxs]{} & b\sigma(g_1) \end{array} \right\} \sqcup \left\{ \begin{array}{ccc} g & \xrightarrow{x} & b\sigma(g) \\ {\scriptstyle s}\downarrow & \overset{sx}{\nearrow} & \downarrow{\scriptstyle s} \\ g_1 & \xrightarrow[sx]{} & b\sigma(g_1) \end{array} \right\}$$

Since we have $\ell(sx) < \ell(x)$, the natural morphism

$$X_1 \to X_1' = \{\ g_1 \xrightarrow{sx} g_2 \xrightarrow{s} b\sigma(g_1),\quad g_1 \xrightarrow{sxs} b\sigma(g_1)\ \}$$

is a universal homeomorphism (note that the composition of $X_1 \to X_1'$ with the projection to g_2 is the map $g \mapsto b\sigma(g)$).
Now we distinguish between the two cases. In case (1), $X_2 = \emptyset$, and applying the proposition once more, we find that in this case the projection

$$X_1' = \{\ g_1 \xrightarrow{sx} g_2 \xrightarrow{s} b\sigma(g_1),\quad g_1 \xrightarrow{sxs} b\sigma(g_1)\ \} \longrightarrow \{\ g_1 \xrightarrow{sxs} b\sigma(g_1)\ \} = X_{sxs}(b)$$

is an isomorphism.
Next we come to case (2). The projection

$$X_1' = \{\ g_1 \xrightarrow{sx} g_2 \xrightarrow{s} b\sigma(g_1),\quad g_1 \xrightarrow{sxs} b\sigma(g_1)\ \} \longrightarrow \{\ g_1 \xrightarrow{sxs} b\sigma(g_1)\ \} = X_{sxs}(b)$$

has fibers of dimension $\frac{1}{2}(\ell(sx) + \ell(s) - \ell(sxs)) = 1$, which proves the claim about X_1. Furthermore X_2 can be replaced with

$$X_2' = \{\ g_1 \xrightarrow{sx} g_2 \xrightarrow{s} b\sigma(g_1),\quad g_1 \xrightarrow{sx} b\sigma(g_1)\ \}$$

up to a universal homeomorphism, and X_2' projects to $X_{sx}(b)$ with 1-dimensional fibers. The corollary is proved. □

With slightly more care, one can show that in case (2) of the lemma, the fibers of the projection $X_1 \to X_{sxs}(b)$ are all isomorphic to $\mathbb{A}^1$, whereas the fibers of $X_2 \to X_{sx}(b)$ are $\mathbb{A}^1 \setminus \{0\}$. This reflects the properties discussed at the end of subsection 2.4.

Lemma 2.5.4. *Let $x, \tau \in \tilde{W}$ with $\ell(\tau) = 0$. Then for any $b \in G(L)$, $X_x(b)$ is isomorphic to $X_{\tau x \tau^{-1}}(b)$.*

Proof. Notice that $X_x(b) = \{gI; g^{-1}b\sigma(g) \in IxI\}$. Thus the isomorphism $G(L)/I \to G(L)/I$, $gI \mapsto gI\tau^{-1} = g\tau^{-1}I$ gives an isomorphism from $X_x(b)$ to $\{gI; (g\tau)^{-1}b\sigma(g\tau) \in IxI\} = \{gI; g^{-1}b\sigma(g) \in \tau IxI\sigma(\tau)^{-1} = I\tau x\tau^{-1}I\} = X_{\tau x\tau^{-1}}(b)$. □

Applying this lemma and the conjugation steps in the reduction method of Deligne and Lusztig, we obtain:

Corollary 2.5.5. *Let $x, x' \in \tilde{W}$, $b \in G(L)$. If $x \tilde{\to} x'$, and $X_{x'}(b) \neq \emptyset$, then $X_x(b) \neq \emptyset$ and $\dim(X_x(b)) - \dim(X_{x'}(b)) \geqslant \frac{1}{2}(\ell(x) - \ell(x'))$.*

2.6

In the sequel, we often use the following property of the Bruhat order: if $\alpha \in \Phi^+$ with corresponding reflection s_α, and $w \in W$, then

$$ws_\alpha > w \text{ if and only if } w\alpha > 0.$$

For further reference, we state the following version of the usual criterion for length additivity.

Lemma 2.6.1. *Let $w, y \in W$ such that $w\alpha < 0$ for every $\alpha \in \Phi^+$ with $y^{-1}\alpha < 0$. Then $\ell(wy) = \ell(w) - \ell(y)$.*

3 Proof of Reuman's conjecture

3.1 Outline of the proof

We first state the result and give an outline of our strategy. Throughout this chapter, we fix $b \in G(L)$, and we assume that whenever we consider $X_x(b)$, then x and b are in the same connected component of $G(L)$.
We consider the following maps from the extended affine Weyl group $\widetilde{W}$ to the finite Weyl group W:

$$\eta_1 \colon \widetilde{W} = X_*(T) \rtimes W \to W, \text{ the projection} \tag{1}$$

$$\eta_2, \text{ where } \eta_2(x) \text{ is the unique element } v \text{ such that } v^{-1}x \in {}^S\widetilde{W} \tag{2}$$

$$\eta(x) = \eta_2(x)^{-1}\eta_1(x)\eta_2(x). \tag{3}$$

So if $x = vt^\mu w$ with μ dominant, $v \in W$, $w \in {}^{I(\mu)}W$, then $\eta_1(x) = vw$, $\eta_2(x) = v$, and $\eta(x) = wv$. Furthermore, for $x \in \widetilde{W}$ (as always, in the same "connected component" as the fixed $b \in G(L)$) we define the *virtual dimension*:

$$d(x) = \frac{1}{2}\big(\ell(x) + \ell(\eta(x)) - \operatorname{def}(b)\big).$$

As discussed above, it is conjectured in [5] that $\dim X_x(b) = d(x)$ for b basic, $x \in \tilde{W}'$ with $X_x(b) \neq \emptyset$.
We denote by w_0 the longest element in W.

Theorem 3.1.1. *Let $x \in \tilde{W}$ and assume that $\eta_2(x) = w_0$ or that the translation part of x is given by a regular coweight. Then* $\dim(X_x(b)) \leqslant d(x)$.

Theorem 3.1.2. *Assume that b is basic. Let $x \in \widetilde{W}'$ such that* $\operatorname{supp}(\eta(x)) = S$. *Then $X_x(b) \neq \emptyset$.*

This proves the non-emptiness statement in Conjecture 9.5.1 (a) of [5]. Together with op. cit., Proposition 9.5.4, which states that the converse of the theorem holds as well, this completely settles the emptiness versus non-emptiness question for basic b and x in the shrunken Weyl chambers $\tilde{W}'$. The next theorem proves that the dimension of $X_x(b)$ is at least as large as predicted by the conjecture if $x \in \tilde{W}'$, and G is a classical group and $b = 1$ or G is of type A_n:

Theorem 3.1.3. *(1) Let G be a classical group, $x \in W_a$ such that* $\mathrm{supp}(\eta(x)) = S$. *If moreover, $x \in \tilde{W}'$ or $\eta(x)$ is a Coxeter element of W, then* $\dim X_x(1) \geqslant d(x)$.
(2) Let $G = PGL_n$ and $\tau \in \widetilde{W}$ with $\ell(\tau) = 0$. Let $x \in W_a\tau$ such that $\mathrm{supp}(\eta(x)) = S$. *If moreover, $x \in \tilde{W}'$ or $\eta(x)$ is a Coxeter element of W, then* $\dim X_x(\tau) \geqslant d(x)$.

The idea of the proofs of these theorems is to relate the given element x to other elements for which non-emptiness, a lower bound on the dimension, or an upper bound on the dimension, respectively, are known. These relations will mainly be shown using the reduction method of Deligne and Lusztig. To this end, we introduce the following notation:

Definition 3.1.4. *Let $x, y \in \widetilde{W}$ such that x, y are in the same W_a-coset. We write $x \Rightarrow y$ if for every b,*

$$\dim X_x(b) - d(x) \geqslant \dim X_y(b) - d(y).$$

Here by convention, we set the dimension of the empty set to be $-\infty$. If the right hand side is $-\infty$ then the inequality holds regardless of the left hand side. In the definition (and in the theorem below) we do not assume that b is basic. This is consistent with the expectation that whenever $x \in \tilde{W}'$ and $X_x(b) \neq \emptyset$, the difference $\dim X_x(b) - d(x)$ is a constant depending only on b, but not on x.
Note that this relation is transitive: If $x \Rightarrow y$, $y \Rightarrow z$, then $x \Rightarrow z$. By definition, if $x \Rightarrow y$ and $X_y(b) \neq \emptyset$, then $X_x(b) \neq \emptyset$. In this case, the lower bound $\dim X_y(b) \geqslant d(y)$ implies the analogous bound for x, while the validity of the upper bound $\dim X_x(b) \leqslant d(x)$ implies the corresponding statement for y. We prove the following statements about the relation $\Rightarrow$:

Theorem 3.1.5.

1. *Let μ be a dominant coweight, $v \in W$ and $w \in {}^{I(\mu)}W$. Assume that $v = w_0$ or that μ is regular. Then*

$$w_0 t^\mu \Rightarrow v t^\mu w.$$

2. *Let $a \in W$ with* $\mathrm{supp}(a) = S$, *and let $\mu \neq 0$ be a dominant coweight. Then there exists a Coxeter element $c \in W$ such that*

$$a t^\mu \Rightarrow t^\mu c.$$

3. *Assume that $x \in \tilde{W}'$, and that* $\mathrm{supp}(\eta(x)) = S$. *Then there exist a dominant coweight λ and $a \in W$ with* $\mathrm{supp}(a) = S$ *such that*

$$x \Rightarrow a t^\lambda.$$

4. *Assume that G is a classical group and $x \in W_a$ with $\eta(x)$ a Coxeter element of W, then*

$$x \Rightarrow \eta(x).$$

Now the non-emptiness statement in Theorem 3.1.2 follows from Theorem 3.1.5 (2) & (3) and the following lemma (Lemma 9.3.3 in [5]), because Coxeter elements obviously are cuspidal.

Lemma 3.1.6. *Let $\mu \in Y$, and let $w \in W$ be a cuspidal element (i. e. the conjugacy class of w does not meet any standard parabolic subgroup), let $x = t^\mu w$, and let b be basic with $\kappa_G(b) = \kappa_G(x)$. Then x is σ-conjugate to b, and in particular $X_x(b) \neq \emptyset$.*

The upper bound on the dimension stated in Theorem 3.1.1 follows from Theorem 3.1.5 (1) and the following lemma:

Lemma 3.1.7. *Let $x = w_0 t^\mu$, where μ is a dominant coweight. Then $\dim X_x(b) \leqslant d(x)$.*

Proof. By the dimension formula for affine Deligne-Lusztig varieties in the affine Grassmannian (see [4], [14]), we have

$$\dim X_\mu(b) = \langle \rho, \mu - \nu_b \rangle - \frac{1}{2}\operatorname{def}(b),$$

where $X_\mu(b)$ denotes the affine Deligne-Lusztig variety in the affine Grassmannian, and ν_b denotes the (dominant) Newton vector of b. Since b is basic, its Newton vector is central and hence does not actually contribute anything. On the other hand, denoting by $\pi\colon$ Flag $\to$ Grass the projection, we have

$$\pi^{-1}(X_\mu(b)) = \bigcup_{x \in W t^\mu W} X_x(b).$$

Therefore, for all $w_1, w_2 \in W$

$$\begin{aligned}\dim X_{w_1 t^\mu w_2}(b) &\leqslant \dim X_\mu(b) + \dim(G/B) = \langle \rho, \mu \rangle - \frac{1}{2}\operatorname{def}(b) + \ell(w_0) \\ &= \frac{1}{2}(\ell(w_0 t^\mu) + \ell(w_0) - \operatorname{def}(b)) = d(w_0 t^\mu).\end{aligned}$$

□

To prove the lower bound under the additional assumptions in Theorem 3.1.3 (1), we reduce to an element of the finite Weyl group. In fact, the following lemma (for $\tau = \mathrm{id}$) shows that it suffices to prove that $x \Rightarrow c$ for some element $c \in W$. If $\eta(x)$ is a Coxeter element, then this follows immediately from Theorem 3.1.5 (4). On the other hand, suppose $x \in \tilde{W}'$ and $\operatorname{supp}(\eta(x)) = S$. We apply Theorem 3.1.5 (3). If the coweight λ is $= 0$, then we are done. Otherwise, we can use Theorem 3.1.5 (2) to see that there exists a dominant coweight λ and a Coxeter element $c \in W$ such that $x \Rightarrow t^\lambda c$. Writing $t^\lambda c = v_1 t^\nu v_2$ with $t^\nu v_2 \in {}^S\tilde{W}$, i. e. $\eta_2(t^\lambda c) = v_1$, we have $c = v_1 v_2$ and $\eta(t^\lambda c) = v_2 v_1$. Since $c = v_1 v_2$ is simply the decomposition into an element of $W_{I(\mu)}$ and an element of ${}^{I(\mu)}W$, we have $\ell(v_1) + \ell(v_2) = \ell(c)$ and since c is a Coxeter element, $v_2 v_1$ is also a Coxeter element of W. Therefore $x \Rightarrow t^\lambda c \Rightarrow v_2 v_1$ (using Theorem 3.1.5 (4)).

Lemma 3.1.8. *Let $\tau \in \widetilde{W}$ with $\ell(\tau) = 0$. Let $J \subset S$ with $\tau(J) = J$. Then for any $w \in W_J$, $\dim X_{w\tau}(\tau) = \ell(w)$.*

Proof. By [9, Lemma 9.7], $\dim X_{w\tau}(\tau) = \dim X_\tau(\tau) + \ell(w)$. By [9, Prop 10.3], $\dim X_\tau(\tau) = 0$. So $\dim X_{w\tau}(\tau) = \ell(w)$. □

Under the assumption in Theorem 3.1.3 (2), we have that $\tau = 1$ or $0 < r < n$ and that τ is the length 0-element that corresponds to the r-th fundamental coweight of G. The case that $\tau = 1$ is included in Theorem 3.1.3 (1). So we only need to consider the latter case. Similarly to the proof above, we have that $x \Rightarrow t^\lambda c$ for some Coxeter element c of W. Let $m = \gcd(n, r)$. Then by [9, Prop 6.7 (2)], $t^\lambda c \tilde{\to} (12 \cdots m)\tau$. Hence by Corollary 2.5.5 and the Lemma above,

$$\begin{aligned}\dim X_{t^\lambda c}(\tau) &\geqslant \dim X_{(12\cdots m)\tau}(\tau) + \frac{1}{2}(\ell(t^\lambda c) - \ell((12\cdots m)\tau)) \\ &= \frac{1}{2}(\ell(t^\lambda c) + m - 1).\end{aligned}$$

Since c is a Coxeter element, $\eta(t^\lambda c)$ is also a Coxeter element of W. We also have that $\operatorname{def}(\tau) = n - m$. Thus $d(t^\lambda c) = \frac{1}{2}(\ell(t^\lambda c) + n - 1 - \operatorname{def}(\tau)) = \frac{1}{2}(\ell(t^\lambda c) + m - 1) \leqslant \dim X_{t^\lambda c}(\tau)$. So we obtain $d(x) \leqslant \dim X_x(\tau)$.
Therefore it remains to prove Theorem 3.1.5. This is the goal of the following sections.

3.2 Reduction of virtual dimension

Lemma 3.2.1. *If $x, x' \in \tilde{W}$ such that $x \tilde{\to} x'$ and $\ell(\eta(x)) = \ell(\eta(x'))$, then $x \Rightarrow x'$.*

Proof. Since $\ell(\eta(x)) = \ell(\eta(x'))$, we have $d(x) - d(x') = \frac{1}{2}(\ell(x) - \ell(x'))$. The Lemma now follows immediately from Corollary 2.5.5. □

Lemma 3.2.2. *Let $x \in \widetilde{W}$. Let $s \in S$ be a simple reflection such that $\ell(sxs) = \ell(x) - 2$. Then*

$$d(x) \geqslant d(sx) + 1,$$

and equality holds if and only if $\ell(\eta(sx)) = \ell(\eta(x)) - 1$.

Proof. We write x as $vt^\mu w$ with $v, w \in W$ and μ a dominant coweight such that $t^\mu w \in {}^S\tilde{W}$. Then $\eta(x) = wv$.
Since $sx < x$, we must have that $sv < v$. If $ws < w$, then $t^\mu ws \in {}^S\tilde{W}$ and $xs > x$, which is a contradiction. Therefore $ws > w$. Let α denote the simple root corresponding to s, and write $\beta = v^{-1}(-\alpha)$, which is a positive root because $sv < v$. We then have $wv(\beta) = w(-\alpha) < 0$ (since $ws > w$), and obtain

$$\eta(sx) = wsv = wvs_\beta < wv,$$

as desired. □

Similarly,

Lemma 3.2.3. *Let $x = vt^\mu w$ with $v, w \in W$ and μ a dominant coweight such that $t^\mu w \in {}^S\tilde{W}$. Let $s \in S$ be a simple reflection such that $\ell(sxs) = \ell(x) - 2$.*

1. *We have $d(x) = d(xs) + 1$ if and only if $\ell(\eta(xs)) = \ell(\eta(x)) - 1$.*
2. *If $t^\mu ws \in {}^S\tilde{W}$ or $w = 1$, then*

$$d(x) \geqslant d(xs) + 1.$$

These results about the virtual dimension imply

Lemma 3.2.4. *Let $x \in \tilde{W}$, $s \in S$ such that $\ell(sxs) < \ell(x)$. Then*

1. *If $\ell(\eta(sx)) = \ell(\eta(x)) - 1$, then $x \Rightarrow sx$.*
2. *If $\ell(\eta(xs)) = \ell(\eta(x)) - 1$, then $x \Rightarrow xs$.*

Proof. For (1), we simply use the Deligne-Lusztig reduction (where we consider X_2 in Corollary 2.5.3 (2)), and Lemma 3.2.2. For part (2), we first use the Deligne-Lusztig reduction from x to sx as in the first case. Then we use Corollary 2.5.3 (1) to reduce to $xs = s(sx)s$ which has the same length as sx. Altogether we see that if $X_{xs}(b) \neq \emptyset$, then $X_x(b) \neq \emptyset$, and, using Lemma 3.2.3 (1),

$$\dim X_x(b) - \dim X_{xs}(b) \geqslant 1 = d(x) - d(xs).$$

□

3.3 Proof of Theorem 3.1.5 (1)

We write $x = vt^\mu w$. First consider the case $v = \eta_2(x) = w_0$. Then we have that $w_0 t^\mu \Rightarrow x = w_0 t^\mu w$ because we can successively apply Lemma 3.2.4 (2). Now we consider the case that μ is regular. Since μ is regular, $t^\mu wvw_0 \in {}^S\tilde{W}$, so we can apply the "$\eta_2 = w_0$"-case to the element $w_0 t^\mu wvw_0$ and obtain that $w_0 t^\mu \Rightarrow w_0 t^\mu wvw_0$. Because μ is regular, Lemma 3.2.1 shows that

$$w_0 t^\mu wvw_0 = w_0 v^{-1}(vt^\mu w)vw_0 \Rightarrow vt^\mu w = x.$$

3.4 Proof of Theorem 3.1.5 (2)

We prove the following stronger result:
Let $J \subset S$ and $x = vt^\mu w$ with $v, w \in W$, $\text{supp}(v) = J$, w is a Coxeter element in W_{S-J}, $\mu \neq 0$ and $t^\mu w \in {}^S\tilde{W}$. Then there exists a Coxeter element c of W such that $vt^\mu w \Rightarrow t^\mu c$.
We proceed by induction on $|J|$. Suppose that the statement is true for all $J' \subsetneq J$, but not true for J. We may also assume that the claim of the proposition

is true for all v' with support $\operatorname{supp}(v') = J$ and $\ell(v') < \ell(v)$. Let $v = s_{i_1} \cdots s_{i_k}$ be a reduced expression.
If $t^\mu w s_{i_1} \in {}^S\tilde{W}$, then $\ell(t^\mu w s_{i_1}) = \ell(t^\mu) - \ell(w s_{i_1}) = \ell(t^\mu) - \ell(w) - 1 = \ell(t^\mu w) - 1$ and $\ell(s_{i_1} v t^\mu w s_{i_1}) = \ell(s_{i_1} v) + \ell(t^\mu w s_{i_1}) = \ell(s_{i_1} v) + \ell(t^\mu w) - 1 = \ell(v t^\mu w) - 2$. By Lemma 3.2.4 (1), $v t^\mu w \Rightarrow s_{i_1} v t^\mu w$. If $\operatorname{supp}(s_{i_1} v) = J$, then by induction, there exists a Coxeter element c of W such that $s_{i_1} v t^\mu w \Rightarrow t^\mu c$. Hence $v t^\mu w \Rightarrow t^\mu c$. That is a contradiction.
Now suppose that $t^\mu w s_{i_1} \in {}^S\tilde{W}$, but $\operatorname{supp}(s_{i_1} v) \subsetneq J$. In that case, we have $\ell(s_{i_1} v t^\mu w s_{i_1}) = \ell(v t^\mu w) - 2$. So $v t^\mu w \Rightarrow s_{i_1} v t^\mu w s_{i_1}$ by Lemma 3.2.1. That is also a contradiction by induction hypothesis.
Now we can assume that $t^\mu w s_{i_1} \notin {}^S\tilde{W}$. Then we have that $t^\mu w s_{i_1} = s_{i'_1} t^\mu w$ for some $i'_1 \in S$. So $w s_{i_1} w^{-1} = t^{-\mu} s_{i'_1} t^\mu$ is a reflection in W. So t^μ commutes with $s_{i'_1}$ and $w s_{i_1} w^{-1} = s_{i'_1}$ is a simple reflection. By our assumptions on w, it follows that $i'_1 = i_1$ and $t^\mu w$ commutes with s_{i_1}. In this case, if $\ell(s_{i_1} v s_{i_1}) < \ell(v)$, then $\operatorname{supp}(s_{i_1} v) = J$ and using Lemma 3.2.4 (1) and the induction hypothesis as in the first case, we again have that $v t^\mu w \Rightarrow t^\mu c$ for some Coxeter element c of W, which is a contradiction.
Therefore we must have that s_{i_1} commutes with $t^\mu w$ and $\ell(s_{i_1} v s_{i_1}) = \ell(v)$. In this case, $v t^\mu w \approx s_{i_1} v s_{i_1} t^\mu w$. So $\dim X_{v t^\mu w}(b) = \dim X_{s_{i_1} v s_{i_1} t^\mu w}(b)$ by Corollary 2.5.3 (1). We also have $d(v t^\mu w) = d(s_{i_1} v s_{i_1} t^\mu w)$, because $\eta(s_{i_1} v s_{i_1} t^\mu w) = w s_{i_1} v s_{i_1}$ has length $\ell(w) + \ell(s_{i_1} v s_{i_1})$ (use that w is a Coxeter element in W_{S-J}). Applying the same argument to $s_{i_1} v s_{i_1} t^\mu w$ instead of $v t^\mu w$, we have that s_{i_2} commutes with $t^\mu w$. Repeating the same procedure, one can show that s_{i_j} commutes with $t^\mu w$ for all $1 \leqslant j \leqslant k$. In particular, s_k commutes with w for all $k \in J$. Since G is quasi-simple, this is only possible if $J = \emptyset$ or $J = S$. If $J = \emptyset$, then $v = 1$ and w is a Coxeter element of W and the statement automatically holds. If $J = S$, then s_i commutes with t^μ for all $i \in S$. Thus $\mu = 0$, which contradicts our assumption.

3.5 Proof of Theorem 3.1.5 (3)

Let $x = v t^\mu w \in \tilde{W}'$ with $\mu \in Y_+$, $v \in W$, $w \in {}^{I(\mu)}W$. We first give the definition of the elements γ and a that we use. Let $J = \{i \in S; s_i w < w\}$. Since $w \in {}^{I(\mu)}W$, $J \cap I(\mu) = \emptyset$. Hence $\mu - \rho_J^\vee \in Y_+$. By definition, $\langle \rho_J^\vee, \alpha_i \rangle - \delta_{w^{-1}\alpha_i} = 0$ for any $i \in S$. Since $x \in \tilde{W}'$, we obtain $\langle \mu - \rho_J^\vee, \alpha_i \rangle + \delta_{v\alpha_i} \neq 0$ for any $i \in S$. Let $J' = I(\mu - \rho_J^\vee)$. Then $v\alpha_i < 0$ for any $i \in J'$. Thus $v = v' w_{J'}^0$ for some $v' \in W^{J'}$. Here $w_{J'}^0$ is the largest element in $W_{J'}$. Now $wv = (wv') w_{J'}^0 = w' z$ for some $w' \in W^{J'}$ and $z \in W_{J'}$. Define $\gamma \in Y_+$ and $y \in W^{I(\gamma)}$ by $\mu - \rho_J^\vee + (w')^{-1} \rho_J^\vee = y\gamma$. Furthermore, we define $a = (y^{-1} z) * (w' y)$. It has support $\operatorname{supp}(a) = S$ since $S = \operatorname{supp}(wv) \subseteq \operatorname{supp}(w'y) \cup \operatorname{supp}(y^{-1} z)$.
We show that
(A) $\ell(w'y) = \ell(w') - \ell(y)$.
Let $\alpha \in \Phi^+$ with $y^{-1}\alpha < 0$. Then $\langle \gamma, y^{-1}\alpha \rangle \leqslant 0$. If $\langle \gamma, y^{-1}\alpha \rangle = 0$, then $y^{-1}\alpha \in \Phi^-_{I(\gamma)}$ and $\alpha = y(y^{-1}\alpha) \in \Phi^-$. That is a contradiction. Hence $\langle \mu - \rho_J^\vee +$

$(w')^{-1}\rho_J^\vee, \alpha\rangle = \langle y\gamma, \alpha\rangle = \langle \gamma, y^{-1}\alpha\rangle < 0$. Since $\mu - \rho_J^\vee \in Y_+$, $\langle \mu - \rho_J^\vee, \alpha\rangle \geqslant 0$. Thus $\langle \rho_J^\vee, w'\alpha\rangle = \langle (w')^{-1}\rho_J^\vee, \alpha\rangle < 0$ and $w'\alpha < 0$. Since $w'\alpha < 0$ for any $\alpha \in \Phi^+$ with $y^{-1}\alpha < 0$, Lemma 2.6.1 shows that $\ell(w'y) = \ell(w') - \ell(y)$. (a) is proved.

Now set $x_1 = vz^{-1}t^{\mu-\rho_J^\vee}y$ and $x_2 = y^{-1}zt^{\rho_J^\vee}w$. Then $x = x_1x_2$ and we claim that

(b) $\ell(x) = \ell(x_1) + \ell(x_2)$.

By the proof of (a), $y \in {}^{J'}W$. In fact, if for any $j \in J'$, $y^{-1}\alpha_j < 0$, then by the proof of (a), $w'\alpha_j < 0$, which contradicts that $w' \in W^{J'}$. Hence $t^{\mu-\rho_J^\vee}y \in {}^S\tilde{W}$ and $\ell(x_1) = \ell(vz^{-1}) + \ell(t^{\mu-\rho_J^\vee}) - \ell(y) = \ell(t^{\mu-\rho_J^\vee}) + \ell(v) - \ell(z) - \ell(y)$. Also $\ell(x_2) = \ell(y^{-1}z) + \ell(t^{\rho_J^\vee}) - \ell(w) = \ell(t^{\rho_J^\vee}) + \ell(y) + \ell(z) - \ell(w)$. Thus $\ell(x_1) + \ell(x_2) = \ell(t^{\mu-\rho_J^\vee}) + \ell(t^{\rho_J^\vee}) + \ell(v) - \ell(w) = \ell(t^\mu) + \ell(v) - \ell(w) = \ell(x)$. (b) is proved.

Now

$$X_x(b) = \{\, g \xrightarrow{x} b\sigma(g) \,\} = \{\, g \xrightarrow{x_1} g_1 \xrightarrow{x_2} b\sigma(g) \,\}.$$

Set

$$\begin{aligned} X_1 =& \{\, g_1 \xrightarrow{x_2} g_2 \xrightarrow{x_1} b\sigma(g_1) \,\} \\ \cong& \{\, g_1 \xrightarrow{y^{-1}z} g_3 \xrightarrow{t^{\rho_J^\vee}w} g_2 \xrightarrow{x_1} b\sigma(g_1) \,\}. \end{aligned}$$

The map $(g, g_1) \mapsto (g_1, b\sigma(g))$ is a universal homeomorphism from $X_x(b)$ to X_1. Let

$$X_2 = \{\, g_1 \xrightarrow{y^{-1}z} g_3 \xrightarrow{t^{\rho_J^\vee}w} g_2 \xrightarrow{x_1} b\sigma(g_1),\ g_3 \xrightarrow{w'yt^\gamma} b\sigma(g_1) \,\} \subset X_1.$$

Then we have that $\dim(X_x(b)) \geqslant \dim(X_2)$.

Now let

$$X_3 = \{\, g_1 \xrightarrow{y^{-1}z} g_3 \xrightarrow{w'yt^\gamma} b\sigma(g_1) \,\},$$

and let $f : X_2 \to X_3$ be the projection map. Notice that $w'yt^\gamma = t^{\rho_J^\vee}wx_1$. Thus by 2.5.2 (1), the map is surjective and each fiber is of dimension $\frac{\ell(t^{\rho_J^\vee}w)+\ell(x_1)-\ell(w'yt^\gamma)}{2} = \frac{\ell(x)-\ell(y^{-1}z)-\ell(w'y)-\ell(t^\gamma)}{2}$. Hence

(c) $\dim(X_x(b)) \geqslant \dim(X_3) + \frac{\ell(x)-\ell(y^{-1}z)-\ell(w'y)-\ell(t^\gamma)}{2}$.

Notice that

$$X_3 = \{\, g_1 \xrightarrow{y^{-1}z} g_3 \xrightarrow{w'y} g_4 \xrightarrow{t^\gamma} b\sigma(g_1) \,\}.$$

Recall that $a = (y^{-1}z) * (w'y)$. We set

$$X_4 = \{\ \underbrace{g_1 \xrightarrow{y^{-1}z} g_3 \xrightarrow{w'y} g_4}_{a} \xrightarrow{t^{\gamma}} b\sigma(g_1)\ \},$$

$$X_5 = \{\ g_1 \xrightarrow{a} g_4 \xrightarrow{t^{\gamma}} b\sigma(g_1)\ \}.$$

By 2.5.2 (2), $\dim(X_3) \geqslant \dim(X_4) \geqslant \dim(X_5) + \ell(y^{-1}z) + \ell(w'y) - \ell(a)$. As we proved above, $\ell(y^{-1}z) + \ell(w'y) = \ell(w') + \ell(z) = \ell(wv)$. Therefore $\ell(y^{-1}z) + \ell(w'y) + \frac{\ell(x)-\ell(y^{-1}z)-\ell(w'y)-\ell(t^{\gamma})}{2} = \frac{\ell(x)+\ell(wv)-\ell(t^{\gamma})}{2}$. So

(D) $\dim(X_x(b)) \geqslant \dim(X_5) + \frac{\ell(x)+\ell(wv)-\ell(t^{\gamma})}{2} - \ell(a)$.

Notice that $\ell(at^{\gamma}) = \ell(a) + \ell(t^{\gamma})$. Thus the map $(g_1, g_4) \mapsto g_1$ gives an isomorphism $X_5 \cong X_{at^{\gamma}}(b)$.

If $X_{at^{\gamma}}(b) \neq \emptyset$, then we obtain that $X_x(b) \neq \emptyset$, and

$$\dim X_x(b) \geqslant \dim X_{at^{\gamma}}(b) + d(x) - d(at^{\gamma}),$$

i.e., $x \Rightarrow at^{\gamma}$.

Example 3.5.1. Let us see what the elements a, γ are in the following two special cases:

1. If $v = 1$, then the assumption that $x \in \tilde{W}'$ implies that $J' = \emptyset$. Therefore $w' = w$, $z = y = 1$, so that $\gamma = \mu$ and $a = w$. The result in this case is that $t^{\mu}w \Rightarrow wt^{\mu}$.

2. If μ is "very regular", then $I(\mu) = I(\mu - \rho_J^{\vee} + (w')^{-1}\rho_J^{\vee}) = \emptyset$, so that $a = w' = wv$. In this case we obtain $vt^{\mu}w \Rightarrow wvt^{\gamma}$.

3.6 Proof of Theorem 3.1.5 (4)

Since $\eta(x)$ is a Coxeter element of W, by [9, Prop 6.7 (1)], we have that $x \tilde{\rightarrow} \eta(x)$. By Lemma 3.2.1, $x \Rightarrow \eta(x)$.

4 Remarks on the critical strips

4.1 A sharpened criterion for non-emptiness

We have seen that the non-emptiness of $X_x(b)$ for b basic and $x \in \tilde{W}'$ can be decided by looking at $\eta(x) = \eta_2(x)^{-1}\eta_1(x)\eta_2(x)$. In fact, if $\operatorname{supp}(\eta(x)) \neq S$ and the translation part of x is non-trivial in the sense that it is different from the Newton vector of b, then $X_x(b) = \emptyset$ ([5, Proposition 9.5.4]). If $x \in \tilde{W} \setminus \tilde{W}'$, then the converse is not true anymore, but one could ask whether it would help to check whether $\operatorname{supp}(\eta') = S$ for additional elements $\eta' \in W$ (depending on x), and specifically one could try to replace $\eta_2(x)$ by a different element of W.

The following proposition gives a result in this direction, using the notion of P-alcove introduced in [5]. In the proposition, $\eta_2(x)$ is replaced by an element of the form $s_\alpha\eta_2(x)$, where α depends on x. Recall that whenever x is a P-alcove sufficiently far away from the origin, then $X_x(b) = \emptyset$.
Of course, the proposition is of particular interest, if ${}^xI \cap U_\alpha = I \cap U_\alpha$ (in particular $x \notin \tilde{W}'$, and more specifically, x lies in the "critical strip" attached to α).

Proposition 4.1.1. *Let $x = vt^\mu w \in \widetilde{W}$, $w \in {}^{I(\mu)}W$, let α be a finite root such that ${}^xI \cap U_\alpha \subseteq I \cap U_\alpha$, and assume that $-v^{-1}\alpha$ is a simple root. If there exists $j \in S$ such that*

$$(s_\alpha v)^{-1}\eta_1(x)(s_\alpha v) \in W_{S\setminus\{j\}},$$

then x is a P-alcove for $P = {}^{s_\alpha v}P_0$, $P_0 = M_0N_0$ the standard parabolic subgroup whose Levi component M_0 is generated by $S \setminus \{j\}$.

Proof. As usual, we write $P = MN$ for the Levi decomposition of P, where M is the Levi subgroup containing the fixed maximal torus. By definition of P, $x \in \tilde{W}_M$, so we have to show that ${}^xI \cap U_\beta \subseteq I$ for every root β occurring in N. By assumption, $-v^{-1}\alpha$ is a simple root α_i.
Denote by U the unipotent radical of the fixed Borel subgroup of G. Since the alcove $v^{-1}x$ lies in the dominant chamber, we have ${}^{v^{-1}x}I \cap U \subseteq I$. Furthermore, by our normalization of I with respect to the dominant chamber, we have ${}^v(I \cap U) \subset I$, so altogether we obtain

$$ {}^xI \cap {}^vU \subset I. \tag{4}$$

The set R_N of roots occurring in N is

$$R_N = \{vs_i\gamma = s_\alpha v\gamma;\ \gamma \text{ a root in } N_0\}.$$

We distinguish two cases: If $i \neq j$, i.e., $s_i \in W_M$, then s_i stabilizes the set of roots in N_0, and therefore R_N is the set of roots in ${}^vN_0$. In this case our claim follows from (4).
Now let us consider the case $i = j$, so that $\alpha_i \in R_{N_0}$, and $\alpha = -v\alpha_i = vs_i\alpha_i \in R_N$. For all $\beta \in R_N \setminus \{\alpha\}$, we have $v^{-1}\beta > 0$, so ${}^xI \cap U_\beta \subset I$ by (4), and finally we have ${}^xI \cap U_\alpha \subset I$ by assumption. □

Even though the proposition yields examples of pairs (x, b) for which $X_x(b) = \emptyset$ although $\operatorname{supp}(\eta(x)) = S$, it does not give rise to a sufficient criterion for non-emptiness in the critical strips, as can be shown by examples for $G = SL_4$.

5 An example of an affine Deligne-Lusztig variety which is not equidimensional

5.1

Looking again at the reduction method of Deligne and Lusztig, Corollary 2.5.3, we see that the situation in the affine case, in the shrunken Weyl chambers, is very much different from the classical situation: Whereas in the classical situation we always have $\dim X_1 = \dim X - 1$, $\dim X_2 = \dim X$ (denoting by X the pertinent Deligne-Lusztig variety), in the affine shrunken case for the expected dimensions we have $d(sxs) + 1 = d(x)$, $d(sx) + 1 \leqslant d(x)$ — so the closed part X_1, if non-empty, always should have the same dimension as the affine Deligne-Lusztig variety itself, while the open part has at most this dimension. See the example below for a specific case where this inequality is strict and where one can produce examples of affine Deligne-Lusztig varieties which are not equidimensional.

5.2

To give an example of a non-equidimensional affine Deligne-Lusztig variety, we again use Corollary 2.5.3 (2). Let $x = vt^\mu w \in W_a$ be an element with μ dominant and very regular, and let $s \in S$ such that

1. $\ell(sv) < \ell(v)$, $\ell(ws) > \ell(w)$,
2. $\ell(wsv) < \ell(wv) - 1$,
3. $\operatorname{supp}(wv) = \operatorname{supp}(wsv) = S$.

By (1), we have $\ell(sxs) = \ell(x) - 2$. We also have $\eta(x) = \eta(sxs) = wv$, $\eta(sx) = wsv$. Therefore as in Corollary 2.5.3 (2), we write $X_x(1) = X_1 \cup X_2$, where X_1 is of relative dimension 1 over $X_{sxs}(1)$, and X_2 is of relative dimension 1 over $X_{sx}(1)$.
By the main result and assumption (3), we have

$$\dim X_2 = \dim X_{sx}(1) + 1 = d(sx) + 1 < d(x) = \dim X_x(1),$$

where the $<$ in the second line holds because of (2) and Lemma 3.2.2. (We also see that $\dim X_1 = \dim X$.) Since X_2 is open in $X_x(1)$ and has strictly smaller dimension, $X_x(1)$ cannot be equidimensional.
It remains to find elements v, w, and s that satisfy (1)–(3). But this is easy, for instance for type A_3, we can take

$$v = s_1 s_2, \qquad w = s_1 s_2 s_3 s_2, \qquad s = s_1,$$

so that

$$wv = s_1 s_2 s_3 s_2 s_1 s_2, \qquad wsv = s_1 s_2 s_3.$$

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Bundles, Cohomology and Truncated Symmetric Polynomials

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Abstract. The cohomology of the classifying space $BU(n)$ of the unitary group can be identified with the the ring of symmetric polynomials on n variables by restricting to the cohomology of BT, where $T \subset U(n)$ is a maximal torus. In this paper we explore the situation where $BT = (\mathbb{C}P^\infty)^n$ is replaced by a product of finite dimensional projective spaces $(\mathbb{C}P^d)^n$, fitting into an associated bundle

$$U(n) \times_T (\mathbb{S}^{2d+1})^n \to (\mathbb{C}P^d)^n \to BU(n).$$

We establish a purely algebraic version of this problem by exhibiting an explicit system of generators for the ideal of truncated symmetric polynomials. We use this algebraic result to give a precise descriptions of the kernel of the homomorphism in cohomology induced by the natural map $(\mathbb{C}P^d)^n \to BU(n)$. We also calculate the cohomology of the homotopy fiber of the natural map $E\,\mathrm{S}_n \times_{\mathrm{S}_n} (\mathbb{C}P^d)^n \to BU(n)$.

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1. Introduction

One of the nicest calculations in algebraic topology is that of the cohomology of the classifying space $BU(n)$ of the unitary groups as the ring of symmetric polynomials on n variables (see [3]). In fact the restriction map identifies $H^*(BU(n), \mathbb{Z})$ with the invariants in the cohomology of the classifying space BT of a maximal torus under the action of the Weyl group S_n. This leads to a beautiful description of the cohomology of the flag manifold $U(n)/T$ and more specifically a detailed understanding of the fibration $U(n)/T \to BT \to BU(n)$. In this paper we explore the situation where $BT = (\mathbb{C}P^\infty)^n$ is replaced by a product of finite dimensional projective spaces $(\mathbb{C}P^d)^n$, fitting into an associated bundle

$$U(n) \times_T (\mathbb{S}^{2d+1})^n \to (\mathbb{C}P^d)^n \to BU(n).$$

This requires an analysis of truncated symmetric invariants and in particular a precise description of the kernel $I(n,d)$ of the algebra surjection $H^*(BU(n),\mathbb{F}) \to H^*((\mathbb{C}P^d)^n,\mathbb{F})^{\mathrm{S}_n}$. The purely algebraic version of this problem is studied in §5 and §6. In particular, Theorem 5.1 allows us to exhibit an explicit set of generators for $I(n,d)$ as follows.

THEOREM 1.1. *Let $\mathbb{F}$ be a field and $I(n,d)$ be the kernel of the map $H^*(BU(n),\mathbb{F}) \to H^*((\mathbb{C}P^d)^n,\mathbb{F})$.*
(a) If $n!$ is invertible in $\mathbb{F}$ then $I(n,d)$ is generated by the elements $P_{d+1}, P_{d+2}, \ldots, P_{d+n}$
(b) If $n < 2\,\mathrm{char}(\mathbb{F}) - 1$ then $I(n,d)$ is generated by $P_{d+1}, P_{d+2}, \ldots, P_{d+n}$ and $P_{\underbrace{d+1,\ldots,d+1}_{p\ times}}$.

For the definition of P_{d+i} and $P_{\underbrace{d+1,\ldots,d+1}_{p^i\ \text{times}}}$, see §5. Note that the degree of P_{d+i} is $2(d+i)$ and the degree of $P_{\underbrace{d+1,\ldots,d+1}_{p\ \text{times}}}$ is $2p(d+1)$.

If $n!$ is invertible in a field $\mathbb{F}$, then we show that the elements P_{d+i}, $1 \le i \le n$, form a generating regular sequence for $I(n,d)$. In contrast, using Theorem 6.1 we show that in most other cases $I(n,d)$ cannot be generated by a regular sequence:

THEOREM 1.2. *If $n \ge \mathrm{char}(\mathbb{F}) > 0$ and $d > 1$, then $I(n,d)$ cannot be generated by a regular sequence.*

There is a free action of S_n on the fiber space $W(n,d) = U(n) \times_T (\mathbb{S}^{2d+1})^n$ arising from the normalizer of the maximal torus in $U(n)$. The orbit space $X(n,d)$ can be realized as the fiber of the natural map $E\,\mathrm{S}_n \times_{\mathrm{S}_n} (\mathbb{C}P^d)^n \to BU(n)$. Our algebraic results allow us to calculate the cohomology of this space in good characteristic.

THEOREM 1.3. *If $\mathbb{F}$ is a field where $n!$ is invertible, then the cohomology of $X(n,d)$ is an exterior algebra on n generators*

$$H^*(X(n,d),\mathbb{F}) \cong \Lambda_{\mathbb{F}}(E_{d+1},\ldots,E_{d+n})$$

where E_j is a cohomology class in dimension $2j-1$.

This has an interesting computational consequence.

THEOREM 1.4. *For any field $\mathbb{F}$ of coefficients, the Serre spectral sequence for the fibration $(\mathbb{S}^{2d+1})^n \to W(n,d) \to U(n)/T$ collapses at E_2 if and only if $d \ge n-1$. Consequently, we obtain an additive calculation*

$$H^*(W(n,d),\mathbb{F}) \cong H^*(U(n)/T,\mathbb{F}) \otimes H^*((\mathbb{S}^{2d+1})^n,\mathbb{F})$$

whenever $d \ge n-1$. In particular if $n!$ is invertible in $\mathbb{F}$, then

$$H^*(X(n,d),\mathbb{F}) \cong [H^*(U(n)/T,\mathbb{F}) \otimes H^*((\mathbb{S}^{2d+1})^n,\mathbb{F})]^{\mathrm{S}_n} \cong \Lambda_{\mathbb{F}}(E_{d+1},\ldots,E_{d+n})\,.$$

These results follow from a general theorem about the cohomology of fibrations which, although "classical" in nature, seems to be new.

THEOREM 1.5. *Let $\mathbb{F}$ be a field and let $\pi : E \to B$ denote a fibration with fiber F of finite type such that B is simply connected. Assume*

- *$H^*(B,\mathbb{F})$ is a polynomial algebra on n even dimensional generators,*
- *$\pi^* : H^*(B,\mathbb{F}) \to H^*(E,\mathbb{F})$ is surjective,*
- *the kernel of π^* is generated by a regular sequence $u_1,\dots,u_n$, where $|u_i| = 2r_i$.*

Then $H^*(F,\mathbb{F})$ is an exterior algebra on n odd dimensional generators $e_1,\dots,e_n$, where $|e_i| = 2r_i - 1$.

It is natural to ask whether the results of this paper can be extended to compact Lie groups, other than $U(n)$. We thus conclude this introduction with the following open problem.

PROBLEM: Let G be a compact Lie group with maximal torus T of rank n and Weyl group W. Describe generators for the kernel $I_G(n,d)$ of the natural map $H^*(BG,\mathbb{F}) \to H^*((\mathbb{C}P^d)^n,\mathbb{F})$ and use this to describe the cohomology of the homotopy fiber of $(\mathbb{C}P^d)^n \to BG$ when $|W|$ is invertible in $\mathbb{F}$.

Theorems 5.1(a) and 6.1(a) have been independently proved in a recent preprint [4] by A. Conca, C. Krattenthaler, J. Watanabe. We are grateful to J. Weyman for bringing this preprint to our attention.

2. BUNDLES AND SYMMETRIC INVARIANTS

A classical computation in algebraic topology is that of the cohomology of the classifying space $BU(n)$ where $U(n)$ is the unitary group of $n\times n$ matrices. We briefly recall how that goes; details can be found, e.g., in the survey paper [3] by A. Borel. Let $T = (\mathbb{S}^1)^n \subset U(n)$ denote the maximal torus of diagonal matrices in $U(n)$; its classifying space is $BT = (\mathbb{C}P^\infty)^n$. The inclusion $T \subset U(n)$ induces a map between the cohomology of $BU(n)$ and the cohomology of BT. Note that the normalizer NT of the torus is a wreath product $\mathbb{S}^1 \wr \mathrm{S}_n$, where the symmetric group S_n acts by permuting the n diagonal entries. Thus the Weyl group NT/T is the symmetric group S_n. Recall that $H^*(BT,\mathbb{Z}) \cong \mathbb{Z}[x_1,\dots,x_n]$, where the $x_1,\dots,x_n$ are 2-dimensional generators.

THEOREM 2.1. *The inclusion $T \subset U(n)$ induces an inclusion in cohomology with image the ring of symmetric invariants in the graded polynomial algebra*

$$H^*(BU(n),\mathbb{Z}) \cong H^*(BT,\mathbb{Z})^{\mathrm{S}_n} = \mathbb{Z}[x_1,\dots,x_n]^{\mathrm{S}_n}\,,$$

where the action of S_n arises from that of the Weyl group. □

Now recall that the complex projective space $\mathbb{C}P^d$ is a natural subspace of $\mathbb{C}P^\infty$; this induces a map

$$\tilde{F}(n,d) : (\mathbb{C}P^d)^n \to BT \to BU(n).$$

The permutation matrices $S_n \subset U(n)$ act via conjugation on $U(n)$; this restricts to an action on the diagonal maximal torus T which permutes the factors. Applying the classifying space functor yields actions of S_n on BT and $BU(n)$ which make the map $\tilde{F}(n,d)$ equivariant. Note however that the conjugation action on $U(n)$ is homotopic to the identity on $BU(n)$. We conclude that $\tilde{F}(n,d)$ induces the natural map

$$\tilde{F}(n,d)^* : H^*(BU(n),\mathbb{Z}) \cong \mathbb{Z}[x_1,\dots,x_n]^{S_n} \to \mathbb{Z}[x_1,\dots,x_n]/(x_1^{d+1},\dots x_n^{d+1})$$

in integral cohomology whose image is precisely the ring of truncated symmetric invariants. We should also note that the map $\tilde{F}(n,d)$ is (up to homotopy) the classifying map for the n–fold product of the canonical complex line bundle over $\mathbb{C}P^d$.

To make this effective geometrically, we need to describe the map $\tilde{F}(n,d)$ explicitly as a fibration. The space $(\mathbb{C}P^d)^n$ is a quotient of $(\mathbb{S}^{2d+1})^n$ by the free action of the maximal torus T. Using a standard induction construction we can view our map as a fibration which lies over the classical fibration connecting $U(n)/T$, BT and $BU(n)$. Indeed, the following commutative diagram has fibrations in its rows and columns:

$$\begin{array}{ccccccc}
 & & (\mathbb{S}^{2d+1})^n & = & (\mathbb{S}^{2d+1})^n & & \\
 & & \downarrow & & \downarrow & & \\
W(n,d) & = & U(n) \times_T (\mathbb{S}^{2d+1})^n & \longrightarrow & (\mathbb{C}P^d)^n & \xrightarrow{\tilde{F}(n,d)} & BU(n) \\
 & & \downarrow & & \downarrow & & \| \\
 & & U(n)/T & \longrightarrow & BT & \longrightarrow & BU(n)
\end{array}$$

Note that we also have a bundle

$$U(n) \to U(n) \times_T (\mathbb{S}^{2d+1})^n \to (\mathbb{C}P^d)^n$$

and its classifying map is $\tilde{F}(n,d)$.

In some of our applications it will also make sense to take a quotient by the action of the symmetric group S_n. For technical reasons this requires taking a *homotopy orbit space* which we now define.

Definition 2.2. Let G denote a compact Lie group acting on a space X, its homotopy orbit space X_{hG} is defined as the quotient of the product space $EG \times X$ by the diagonal G–action, where EG is the universal G–space.

Remark 2.3. It should be noted that if G is a finite group, X is a G–space and $|G|$ is invertible in the coefficients, then the natural projection $X_{hG} \to X/G$ induces an isomorphism in cohomology (this follows from the Vietoris-Begle theorem). Hence for example if $|G|$ is invertible in a coefficient field $\mathbb{F}$, then $H^*(X_{hG},\mathbb{F}) \cong H^*(X,\mathbb{F})^G$ (the algebra of invariants).

In our context, the symmetric group S_n acts by permuting the factors in $(\mathbb{C}P^d)^n$ and we can consider the associated homotopy orbit space

$$(\mathbb{C}P^d)^n_{h\,\mathrm{S}_n} = E\,\mathrm{S}_n \times_{\mathrm{S}_n} (\mathbb{C}P^d)^n.$$

More precisely, the map $BT \to BU(n)$ naturally factors through the classifying space of the normalizer NT, as we have $T \subset NT \subset U(n)$. The space BNT can be identified with $BT_{h\,\mathrm{S}_n} = (\mathbb{C}P^\infty)^n_{h\,\mathrm{S}_n}$, where S_n acts by permuting the factors, as before. This homotopy orbit space restricts to the truncated projective spaces, yielding a map

$$F(n,d) : (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n} \to BU(n)\,,$$

which is surjective in rational cohomology. We would also like to describe this map as a fibration.

The map $(\mathbb{C}P^d)^n \to BT$ is an S_n-equivariant fibration, with fiber $(\mathbb{S}^{2d+1})^n$. This arises from the free T–action on the product of spheres, which extends in the usual way to an action of the semidirect product NT. If we take homotopy orbit spaces we obtain a fibration sequence

$$(\mathbb{S}^{2d+1})^n \to (\mathbb{S}^{2d+1})^n_{hNT} \to BNT\,.$$

Dividing out by the free T–action we can identify $(\mathbb{S}^{2d+1})^n_{hNT} \simeq (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n}$. This makes the fiber of the map $(\mathbb{C}P^d)^n_{h\,\mathrm{S}_n} \to BNT$ very explicit. As before, in order to describe the fibration with target $BU(n)$, it suffices to induce up the action on the fiber to a $U(n)$–action by taking the balanced product $Z = U(n) \times_{NT} (\mathbb{S}^{2d+1})^n$. This yields a fibration sequence

$$Z \to Z_{hU(n)} \to BU(n)\,.$$

Note that

$$Z_{hU(n)} \simeq EU(n) \times_{NT} (\mathbb{S}^{2d+1})^n \simeq (\mathbb{S}^{2d+1})^n_{hNT} \simeq (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n}\,,$$

where the last equivalence follows from taking quotients by the free T–action, as before. Our discussion is summarized in the following diagram of fibrations, analogous to the non–equivariant situation:

$$\begin{array}{ccccccc}
 & & (\mathbb{S}^{2d+1})^n & = & (\mathbb{S}^{2d+1})^n & & \\
 & & \downarrow & & \downarrow & & \\
X(n,d) & = & U(n) \times_{NT} (\mathbb{S}^{2d+1})^n & \longrightarrow & E\,\mathrm{S}_n \times_{\mathrm{S}_n} (\mathbb{C}P^d)^n & \xrightarrow{F(n,d)} & BU(n) \\
 & & \downarrow & & \downarrow & & \| \\
 & & U(n)/NT & \longrightarrow & BNT & \longrightarrow & BU(n)
\end{array}$$

Hence we have

PROPOSITION 2.4. *Up to homotopy the map $\tilde{F}(n,d) : (\mathbb{C}P^d)^n \to BU(n)$ is a fibration with fiber the compact simply connected manifold*

$$W(n,d) = U(n) \times_T (\mathbb{S}^{2d+1})^n$$

of dimension equal to $n(n+2d)$. There is a free S_n–action on this manifold, and its quotient

$$X(n,d) = U(n) \times_{NT} (\mathbb{S}^{2d+1})^n$$

is homotopy equivalent to the fiber of $F(n,d) : (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n} \to BU(n)$. □

REMARK 2.5. Note that there are fibrations

$$(\mathbb{S}^{2d+1})^n \to X(n,d) \to U(n)/NT$$

and

$$U(n) \to X(n,d) \to (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n},$$

where the second one is obtained from pulling back the universal $U(n)$ bundle over $BU(n)$ using $F(n,d)$.

One of our main results in this paper will be to calculate the cohomology of the fibers $W(n,d)$ and $X(n,d)$ associated to the fibrations $\tilde{F}(n,d)$ and $F(n,d)$ respectively.

3. COHOMOLOGY CALCULATIONS WHEN $n!$ IS INVERTIBLE

Our standing assumption in this section (unless stated otherwise) will be that $\mathbb{F}$ is a field such that $n!$ is invertible in $\mathbb{F}$, and cohomology will be computed with $\mathbb{F}$–coefficients. A good example is the field $\mathbb{Q}$ of rational numbers. In this situation we have $H^*(X(n,d),\mathbb{F}) \cong H^*(W(n,d),\mathbb{F})^{\mathrm{S}_n}$; it is this cohomology algebra that we will be most interested in.
We begin by considering the limit case $d = \infty$. In this case $X(n,\infty) = U(n)/NT$ and we are looking at the classical fibration

$$U(n)/NT \to BNT \to BU(n)$$

PROPOSITION 3.1. *The map $BNT \to BU(n)$ induces an isomorphism in cohomology and $U(n)/NT$ is $\mathbb{F}$–acyclic.*

Proof. Indeed, both maps in the sequence

$$H^*(BU(n),\mathbb{F}) \to H^*(BNT,\mathbb{F}) \to H^*(BT,\mathbb{F})^{\mathrm{S}_n}$$

are isomorphisms. Since $BU(n)$ is simply connected, this can only happen if $U(n)/NT$ is acyclic. □

Note that this computation is very different from what the cohomology of the flag manifold $U(n)/T$ looks like; when we divide out by the action of the symmetric group all the reduced cohomology vanishes.
We now consider the unstable case of this result, namely when d is finite. This is considerably more interesting, as we know that the cohomology must be non–trivial. This calculation will be a special case of a more general result about the cohomology of fibrations.

Theorem 3.2. *Let $\pi : E \to B$ denote a fibration with fiber F of finite type such that B is simply connected and*

- *$H^*(B, \mathbb{F})$ is a polynomial algebra on n even dimensional generators,*
- *$\pi^* : H^*(B, \mathbb{F}) \to H^*(E, \mathbb{F})$ is surjective,*
- *the kernel of π^* is generated by a regular sequence $u_1, \ldots, u_n$, where $|u_i| = 2r_i$.*

Then $H^*(F, \mathbb{F})$ is an exterior algebra on n odd dimensional generators $e_1, \ldots, e_n$, where $|e_i| = 2r_i - 1$.

Proof. The cohomology of the fiber F in a fibration

$$F \to E \to B$$

can be studied using the Eilenberg–Moore spectral sequence. We refer the reader to [8], Chapter VIII for details. It has the form:

$$E_2^{*,*} = Tor_{H^*(B,\mathbb{F})}(\mathbb{F}, H^*(E, \mathbb{F})).$$

On the other hand, the hypotheses imply that

$$H^*(E, \mathbb{F}) \cong H^*(B, \mathbb{F})/(u_1, \ldots u_n)\,,$$

where $u_1, \ldots, u_n$ form a regular sequence of maximal length in $H^*(B, \mathbb{F})$, a polynomial algebra on n even dimensional generators. In other words the cohomology of B is free and finitely generated over $\mathbb{F}[u_1, \ldots, u_n]$. Thus the spectral sequence simplifies to

$$E_2^{*,*} = Tor_{H^*(B,\mathbb{F})}(\mathbb{F}, H^*(B, \mathbb{F}) \otimes_{\mathbb{F}[u_1,\ldots,u_n]} \mathbb{F}) \cong Tor_{\mathbb{F}[u_1,\ldots,u_n]}(\mathbb{F}, \mathbb{F})$$

This can be computed using the standard Koszul complex, yielding

$$E_2 = \Lambda_{\mathbb{F}}(e_1, \ldots, e_n)\,,$$

where the e_i are exterior classes in degree $2r_i - 1$. There are no further differentials, as the algebra generators for $E_2^{*,*}$ represent non–trivial elements in the cohomology of F which by construction must transgress to the regular sequence $\{u_1, \ldots, u_n\}$ in $H^*(B, \mathbb{F})$ in the Serre spectral sequence for the fibration

$$F \to E \to B.$$

Therefore the Eilenberg–Moore spectral sequence collapses at $E_2 = E_\infty$. Now this algebra is a free graded commutative algebra, hence there are no extension problems and it follows that

$$H^*(F, \mathbb{F}) \cong \Lambda_{\mathbb{F}}(e_1, \ldots, e_n)$$

as stated in the theorem. ☐

We now apply this result to the spaces $X(n, d)$.

Theorem 3.3. *The cohomology of $X(n, d)$ is an exterior algebra on n generators*

$$H^*(X(n, d), \mathbb{F}) \cong \Lambda_{\mathbb{F}}(E_{d+1}, \ldots, E_{d+n})\,,$$

where E_j is a cohomology class in dimension $2j - 1$.

Proof. As observed previously we have a fibration

$$X(n,d) \to (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n} \to BU(n)\,.$$

The Eilenberg–Moore spectral sequence can therefore be applied to compute the cohomology of $X(n,d)$. The map $F(n,d) : (\mathbb{C}P^d)^n_{h\,\mathrm{S}_n} \to BU(n)$ induces a surjection of algebras

$$H^*(BU(n),\mathbb{F}) \to H^*((\mathbb{C}P^d)^n_{h\,\mathrm{S}_n},\mathbb{F}) \to 0$$

which can be identified with the natural map

$$\mathbb{F}[x_1,\dots,x_n]^{\mathrm{S}_n} \to (\mathbb{F}[x_1,\dots,x_n]/(x_1^{d+1},\dots x_n^{d+1}))^{\mathrm{S}_n}.$$

The kernel of this map is precisely the ideal

$$I_{n,d} = (x_1^{d+1},\dots,x_n^{d+1}) \cap \mathbb{F}[x_1,\dots,x_n]^{\mathrm{S}_n}.$$

By Theorem 6.1(a), $I_{n,d}$ is generated by a regular sequence of elements $P_{d+1},\dots,P_{d+n}$. Here each P_j is a homogeneous polynomial in $x_1,\dots,x_n$ of degree j; its degree as a cohomology class is $2j$. These classes form a regular sequence of maximal length in the polynomial algebra $H^*(BU(n),\mathbb{F})$. Thus the hypotheses of Theorem 3.2 hold, and the proof is complete. □

Corollary 3.4. *If $d < \infty$, then $X(n,d)$ is a compact, connected, orientable manifold.*

Proof. According to our calculation, for $m = n(n+2d)$ we have $H^m(X(n,d),\mathbb{Q}) \cong \mathbb{Q}$. This is precisely the dimension of the compact manifold $X(n,d) = U(n) \times_{NT} (\mathbb{S}^{2d+1})^n$, whence the result follows. □

Remark 3.5. Note that as d gets large, the connectivity of the space $X(n,d)$ increases; this is consistent with the stable calculation, namely the acyclicity of $U(n)/NT$. Also note that the manifold $U(n)/NT$ is not orientable, as it is $\mathbb{Q}$–acyclic.

For the case of $W(n,d)$ we offer the following general result:

Theorem 3.6. *For any field $\mathbb{F}$ of coefficients, the Serre spectral sequence for the fibration $(\mathbb{S}^{2d+1})^n \to W(n,d) \to U(n)/T$ collapses at E_2 if and only if $d \geq n-1$, from which we obtain an additive calculation*

$$H^*(W(n,d),\mathbb{F}) \cong H^*(U(n)/T,\mathbb{F}) \otimes H^*((\mathbb{S}^{2d+1})^n,\mathbb{F}).$$

In particular if $n!$ is invertible in $\mathbb{F}$, then

$$H^*(X(n,d),\mathbb{F}) \cong [H^*(U(n)/T,\mathbb{F}) \otimes H^*((\mathbb{S}^{2d+1})^n,\mathbb{F})]^{\mathrm{S}_n} \cong \Lambda_{\mathbb{F}}(E_{d+1},\dots,E_{d+n})\,.$$

Proof. Consider the Serre spectral sequence with $\mathbb{F}$ coefficients for the fibration $(\mathbb{S}^{2d+1})^n \to W(n,d) \to U(n)/T$. The base is simply connected and the cohomology of the fiber is generated by the natural generators for the $2d+1$–dimensional cohomology of each sphere. The first differential in the spectral sequence can be computed as follows: if $e_i \in H^{2d+1}((\mathbb{S}^{2d+1})^n,\mathbb{F})$ is a natural generator then

$$d_{2d+2}(e_i) = [x_i^{d+1}] \in H^*(U(n)/T,\mathbb{F}) \cong H^*(BT,\mathbb{F})/(s_1,s_2,\dots,s_n)\,,$$

where the $s_1, s_2, \ldots, s_n$ are the symmetric polynomials. This follows from the diagram of fibrations in the previous section and the well-known calculation of the cohomology of $(\mathbb{C}P^d)^n$ and $U(n)/T$ as quotients of $H^*(BT, \mathbb{F})$. We now need the following algebraic lemma.

Lemma 3.7. *Let $\mathbb{F}$ be a commutative ring and I be the ideal of $\mathbb{F}[x_1, ..., x_n]$ generated by the elementary symmetric polynomials $s_1, ..., s_n$ in $x_1, ..., x_n$. Then (a) $x_1^n \in I$ but (b) $x_1^{n-1} \notin I$.*

Suppose Lemma 3.7 is established (we only need it in the case where $\mathbb{F}$ is a field). Then we conclude that $d_{2d+2}(e_i) = [x_i^{d+1}] = 0$ in $H^*(U(n)/T, \mathbb{F})$ for all $i = 1, \ldots, n$ if and only if $d \geq n-1$. This implies that all the differentials in the spectral sequence are zero and so it collapses at E_2. The assertions of Theorem 3.6 follow from this and Theorem 3.3.

It thus remains to prove Lemma 3.7.

(a) Recall that $x_1, \ldots, x_n$ are, by definition, the roots of the polynomial

$$x^n - x^{n-1}s_1 + x^{n-2}s_2 - ... + (-1)^n s_n = 0\,.$$

Thus $x_1^n = x_1^{n-1}s_1 - x^{n-2}s_2 + ... - (-1)^n s_n$, and since every term in the right hand side lies in I, part (a) follows.

(b) Assume, to the contrary, that

$$x_1^{n-1} = f_1 s_1 + ... + f_n s_n \tag{1}$$

for some polynomials $f_1, ..., f_n \in \mathbb{F}[x_1, \ldots, x_n]$. If such an identity is possible over $\mathbb{F}$, and $\alpha\colon \mathbb{F} \to L$ is a ring homomorphism then, applying α to each of the coefficients of $f_1, \ldots, f_n$, we obtain an identity of the same form over L. Thus, for the purpose of showing that (1) is not possible, we may, without loss of generality, replace $\mathbb{F}$ by L. In particular, we may take L to be the algebraic closure of the field $\mathbb{F}/M$, where M is a maximal ideal of $\mathbb{F}$. After replacing $\mathbb{F}$ by this L, we may assume that $\mathbb{F}$ is an algebraically closed field.

Equating the homogeneous terms of degree $n-1$ on both sides, we see that after replacing $f_1, f_2, \ldots, f_{n-1}$ by their homogeneous parts of degrees $n-2, n-3, \ldots, 0$, respectively, we may assume that $f_n = 0$.

Since $\mathbb{F}$ is an algebraically closed field, $x^n - 1$ factors into a product of linear terms

$$x^n - 1 = (x - \zeta_1)(x - \zeta_2) \cdot \ldots \cdot (x - \zeta_n)\,. \tag{2}$$

for some $\zeta_1, \ldots, \zeta_n \in \mathbb{F}$. (As an aside, we remark that $\zeta_1, \ldots, \zeta_n \in \mathbb{F}$ are distinct if $p = \mathrm{char}(\mathbb{F})$ does not divide n but not in general; at the other extreme, if n is a power of p then $\zeta_1 = \cdots = \zeta_n = 1$.) By (2)

$$s_i(\zeta_1, \ldots, \zeta_n) = (-1)^i \text{ (coefficient of } x^{n-i} \text{ in } x^n - 1) = 0$$

for every $i = 1, \ldots, n-1$. Hence, substituting ζ_i for x_i in (1), and remembering that $f_n = 0$, we obtain $\zeta_1^{n-1} = 0$, i.e., $\zeta_1 = 0$. Since ζ_1 is a root of $x^n - 1 = 0$, we have arrived at a contradiction. This shows that (1) is impossible. The proof of Lemma 3.7 and thus of Theorem 3.6 is now complete. □

Calculations with field coefficients can be pieced together to provide information on the integral cohomology of $X(n,d)$.

PROPOSITION 3.8. *The cohomology ring $H^*(X(n,d),\mathbb{Z})$ has no p–torsion if $p>n$.*

Proof. By our previous results if $p>n$ then

$$\dim_{\mathbb{F}_p} H^*(X(n,d),\mathbb{F}_p)=\dim_{\mathbb{Q}} H^*(X(n,d),\mathbb{Q})=2^n.$$

Hence by the universal coefficient theorem, there can be no p–torsion in the integral cohomology of $X(n,d)$. □

The situation is more complicated if $n\geq p=\mathrm{char}(\mathbb{F})$. In particular, we will show that in this case the kernel $I(n,d)$ of the map $H^*(BU(p),\mathbb{F}_p)\to H^*((\mathbb{C}P^d)^p,\mathbb{F}_p)$ cannot be generated by a regular sequence for any $d\geq 2$ (and, in most cases for $d=1$ as well); see Theorem 6.1(b). We now provide an explicit calculation in the case where $n=d=p=2$.

EXAMPLE 3.9. Consider the map $\tilde{F}(2,1):\mathbb{S}^2\times\mathbb{S}^2\to BU(2)$. Its fiber is

$$W(2,1)=U(2)\times_T(\mathbb{S}^3\times\mathbb{S}^3)$$

which itself fibers over $U(2)/T=\mathbb{S}^2$ with fiber $\mathbb{S}^3\times\mathbb{S}^3$. Hence for dimensional reasons $H^*(W(2,1),\mathbb{Z})\cong H^*(\mathbb{S}^3\times\mathbb{S}^3\times\mathbb{S}^2,\mathbb{Z})$. The S_2–action on this space exchanges the two 3-spheres and applies the antipodal map on $\mathbb{S}^2$. Thus the orbit space $X(2,1)$ will be rationally cohomologous to $\mathbb{S}^3\times\mathbb{S}^5$, as predicted by Theorem 3.3. However, it can be shown that $H^*(X(2,1),\mathbb{F}_2)$ has Poincaré series

$$p(t)=1+t+t^2+t^3+t^5+t^6+t^7+t^8\,.$$

On the other hand, the corresponding Poincaré series for rational cohomology is

$$q(t)=1+t^3+t^5+t^8$$

which accounts for the torsion free classes in the integral cohomology. This example illustrates the presence of 2–torsion in the cohomology of $X(2,1)$. Of course in this case we have $\pi_1(X(2,1))=\mathbb{Z}/2$, which accounts for the classes in degrees one and two in mod 2 cohomology, and by Poincaré duality for the classes in degrees six and seven.

On the other hand, recall that if $H^*(BU(2),\mathbb{F}_2)\cong\mathbb{F}_2[c_2,c_4]$ and $H^*(\mathbb{S}^2\times\mathbb{S}^2,\mathbb{F}_2)\cong\Lambda(u_2,v_2)$ then $\tilde{F}(2,1)^*(c_2)=u_2+v_2$ and $\tilde{F}(2,1)^*(c_4)=u_2v_2$. Thus we see that $\tilde{F}(2,1)^*$ is not surjective and that its kernel is generated by the classes $c_2^2, c_2^3+c_2c_4, c_4^2$. These classes correspond to the symmetric polynomials $P_2=x_1^2+x_2^2$, $P_3=x_1^3+x_2^3$ and $P_{2,2}=x_1^2x_2^2$. Note that if 2 is invertible in the coefficients then

$$P_{2,2}=\frac{P_2^2-(x_1+x_2)P_3+(x_1x_2)P_2}{2}\,,$$

and the third generator is redundant.

More generally, using the algebraic calculations in Theorem 5.1, Theorem 6.1 and Corollary 6.3 we obtain the following.

Theorem 3.10. *Assume that $p \leq n \leq 2p-1$ and $d \geq 2$. Then the kernel of the map induced by $\tilde{F}(n,d)$ in cohomology*

$$\tilde{F}(n,d)^* : H^*(BU(n), \mathbb{F}_p) \to H^*((\mathbb{C}P^d)^n, \mathbb{F}_p)$$

is generated by the following $n+1$ elements:

- P_{d+i}, *where* $1 \leq i \leq n$ *and* $|P_j| = 2j$
- $P_{\underbrace{d+1,\dots,d+1}_{p\ times}}$ *and* $|P_{\underbrace{d+1,\dots,d+1}_{p\ times}}| = 2p(d+1)$

Moreover this kernel cannot be generated by a regular sequence or by fewer than $n+1$ elements. □

4. The orthogonal groups and more calculations at $p=2$

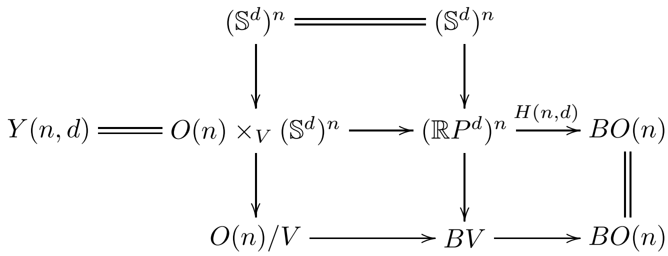
The situation for $p=2$ is somewhat different, as there are specific geometric models which are special to this characteristic. Here we consider the standard diagonal inclusion $V = (\mathbb{Z}/2)^n \hookrightarrow O(n)$ into the group of orthogonal $n \times n$ matrices. The group V is self-centralizing in $O(n)$; its normalizer NV is the wreath product $NV = \mathbb{Z}/2 \wr \mathrm{S}_n$. The Weyl group $W = NV/V$ of V in $O(n)$ is thus isomorphic to S_n; it acts on $V = (\mathbb{Z}/2)^n$ by permuting the n factors of $\mathbb{Z}/2$. The classifying space for V is $BV = (\mathbb{R}P^\infty)^n$, its mod 2 cohomology is a polynomial algebra on n one dimensional generators $\mathbb{F}_2[x_1, \dots, x_n]$. The inclusion induces a map from the cohomology of $BO(n)$ to this algebra, which gives rise to an isomorphism onto the symmetric invariants. As before, the truncated projective space $\mathbb{R}P^d$ is a natural subspace of $\mathbb{R}P^\infty$, and Theorem 5.1 provides a description of the kernel of the homomorphism induced by the map $H(n,d) : (\mathbb{R}P^d)^n \to BO(n)$ for $n = 1, 2, 3$.

The classifying space for $NV = \mathbb{Z}/2 \wr \mathrm{S}_n$ is $BNV = (\mathbb{R}P^\infty)^n_{h\,\mathrm{S}_n}$. However, as our calculations are at $p=2$ and $|\,\mathrm{S}_n\,|$ is even, the homotopy orbit space has a lot more cohomology than just the truncated symmetric invariants (for example, it contains a copy of $H^*(\mathrm{S}_n, \mathbb{F}_2)$). The wreath product NV acts on $(\mathbb{S}^d)^n$ extending the coordinatewise antipodal action of V. Thus we have a fiber bundle $(\mathbb{S}^d)^n \to (\mathbb{R}P^d)^n_{h\,\mathrm{S}_n} \to BNV$, where we identify $(\mathbb{S}^d)^n_{hNV} \simeq (\mathbb{R}P^d)^n_{h\,\mathrm{S}_n}$.

Example 4.1. For $n=2$ we can identify NV with the dihedral group D_8 and its cohomology has generators e, u v in degrees $1, 1, 2$ respectively with the single relation $e \cdot u = 0$ (see [1]). The elements u, v can be identified with the standard symmetric generators $x_1 + x_2$ and $x_1 x_2$ in $H^*(V, \mathbb{F}_2)^{\mathrm{S}_2}$ via the restriction map. In fact we have isomorphisms (see [1], page 118) $H^*(BD_8, \mathbb{F}_2) \cong H^*(\mathrm{S}_2, H^*(V, \mathbb{F}_2))$ and $H^*((\mathbb{S}^d)^2_{hD_8}, \mathbb{F}_2) \cong H^*(\mathrm{S}_2, H^*((\mathbb{R}P^d)^2, \mathbb{F}_2)$. Using these descriptions and Theorem 5.1 it can be shown that the the kernel of the homomorphism $H^*(BD_8, \mathbb{F}_2) \to H^*((\mathbb{S}^d)^2_{hD_8}, \mathbb{F}_2)$ is the ideal generated by the three elements $P_{d+1} = x_1^{d+1} + x_2^{d+2}$, $P_{d+2} = x_1^{d+2} + x_2^{d+2}$ and $P_{d+1,d+1} = x_1^{d+1} x_2^{d+1}$. This ideal is called the Fadell–Husseini index (see [6]) of the D_8–space $\mathbb{S}^d \times \mathbb{S}^d$;

it has some interesting applications in topology and it has been fully calculated in [2].

Geometrically, the fibration which our mod 2 calculations can be applied to is described by the diagram:



Here we recall some classical results. First, from the homotopy long exact sequence of the fibration we see that $O(n)/V$ is path–connected because $\pi_1(BV) \to \pi_1(BO(n)) \cong \mathbb{Z}/2$ is surjective (the dual map in mod 2 cohomology is injective). Its fundamental group acts homologically trivially on $H^*((\mathbb{S}^d)^n, \mathbb{F}_2)$, as it acts through its image in V. Therefore the Serre spectral sequence for the fibration $(\mathbb{S}^d)^n \to Y(n,d) \to O(n)/V$ has the form

$$E_2^{*,*} = H^*(O(n)/V) \otimes H^*((\mathbb{S}^d)^n, \mathbb{F}_2) \implies H^*(Y(n,d), \mathbb{F}_2)\,.$$

Using Lemma 3.7, we see that this spectral sequence collapses at E_2 if and only if $d \geq n-1$.

THEOREM 4.2. *If $d \geq n-1$ then we have an additive isomorphism*

$$H^*(Y(n,d), \mathbb{F}_2) \cong H^*(O(n)/V) \otimes H^*((\mathbb{S}^d)^n, \mathbb{F}_2).$$

□

5. TRUNCATED SYMMETRIC POLYNOMIALS

The remainder of this paper will be devoted to the algebraic results used in the previous sections. Let $\mathbb{F}$ be a field. We begin by recalling some standard notational conventions and facts concerning the ring

$$R_n := \mathbb{F}[x_1, \dots, x_n]^{\mathrm{S}_n}$$

of symmetric polynomials in n variables. For details we refer the reader to [7, Chapter I.2].

If $a_1, \dots, a_n$ are non-negative integers, we will write $P_{a_1,\dots,a_n}$ for the sum of monomials $x^{a_1'} \dots x_n^{a_n'}$, as $a_1', \dots, a_n'$ range over all possible permutations of $a_1, \dots, a_n$. A sum of this form is called a *monomial symmetric function.* It has $\dfrac{n!}{\lambda_1! \cdots \lambda_m!}$ terms, where $\lambda_1, \dots, \lambda_m$ is the partition of n associated to $a_1, \dots, a_n$. (Recall that this means that that there are m distinct integers among $a_1, \dots, a_n$, occurring with multiplicities $\lambda_1, \dots, \lambda_m$, respectively.)

Permuting $a_1, \dots, a_n$ does not change $P_{a_1,\dots,a_n}$, so we will always assume that $a_1 \geq \dots \geq a_n$. With this convention, the monomial symmetric functions $P_{a_1,\dots,a_n}$ form a basis of $R_n := \mathbb{F}[x_1, \dots, x_n]^{\mathrm{S}_n}$ as an $\mathbb{F}$-module. One easily checks that the multiplication rule in this basis is given by

$$P_{a_1,\dots,a_n} \cdot P_{b_1,\dots,b_n} = \sum k_{c_1,\dots,c_n} P_{c_1,\dots,c_n} \,, \tag{3}$$

where $c_1 \geq \ldots \geq c_n$ and there are exactly $k_{c_1,\dots,c_n}$ different ways to write

$$(c_1, \dots, c_n) = (a'_1, \dots, a'_n) + (b'_1, \dots, b'_n)$$

for some permutation $a'_1, \dots, a'_n$ of $a_1, \dots, a_n$ and some permutation $b'_1, \dots, b'_n$ of $b_1, \dots, b_n$.

To make our formulas less cumbersome, we will often abbreviate $P_{a_1,\dots,a_r,0,\dots,0}$ as $P_{a_1,\dots,a_r}$. As long as the number of variables n is fixed, this will not lead to any confusion. For example, in this notation,

$$P_i = x_1^i + \dots + x_n^i$$

is the usual power sum of degree i and

$$\begin{aligned} &P_1 = x_1 + \dots + x_n, \\ &P_{1,1} = x_1x_2 + \dots + x_{n-1}x_n, \\ &\dots \\ &P_{\underbrace{1,\,\dots,\,1}_{n \text{ times}}} = x_1x_2 \dots x_n \end{aligned} \tag{4}$$

are the elementary symmetric polynomials.

The main result of this section is the following theorem.

Theorem 5.1. *Let $\mathbb{F}$ be a field of characteristic $p \geq 0$.*

(a) If $p = 0$ or $n < p$ then the ideal $I_{n,d} := (x_1^{d+1}, \dots, x_n^{d+1}) \cap \mathbb{F}[x_1, \dots, x_n]^{\mathrm{S}_n}$ of $R_n := \mathbb{F}[x_1, \dots, x_n]^{\mathrm{S}_n}$ is generated by $P_{d+1}, \dots, P_{d+n}$.

(b) If $n \leq 2p - 1$ then $I_{n,d}$ is generated by $P_{d+1}, \dots, P_{d+n}$ and $P_{\underbrace{d+1,\,\dots,\,d+1}_{p \text{ times}}}$.

The rest of this section will be devoted to proving Theorem 5.1. Let I be the ideal of $R_n = \mathbb{F}[x_1, \dots, x_n]^{\mathrm{S}_n}$ generated by the polynomials listed in the statement of Theorem 5.1. Clearly, $I \subset I_{n,d}$; we want to prove the opposite inclusion. First we note that every element of $I_{n,d}$ is an $\mathbb{F}$-linear combination of monomial symmetric functions $P_{a_1,\dots,a_n}$, where $a_1 \geq d+1$. Thus in order to prove Theorem 5.1 it suffices to show that every $P_{a_1,\dots,a_n}$ with $a_1 \geq d+1$ lies in I. Our first step in this direction is the following lemma.

We define the *weight* of the monomial symmetric function $P_{a_1,\dots,a_n}$ as the largest integer $r \leq n$ such that $a_r \geq 1$. As mentioned above, we will abbreviate $P_{a_1,\dots,a_n}$ of weight $\leq r$ as $P_{a_1,\dots,a_r}$.

We define the *leading multiplicity* of $P_{a_1,\dots,a_n}$ as the largest integer $s \leq n$ such that $a_1 = \dots = a_s$. Here, as always, we are assuming that $a_1 \geq a_2 \geq \ldots \geq a_n \geq 0$.

Lemma 5.2. *Let $\mathbb{F}$ be a field and $J_{n,d}$ be the ideal of $R_n = \mathbb{F}[x_1, \dots, x_n]^{S_n}$ generated by $P_{d+1}, \dots, P_{d+n}$. Then $J_{n,d}$ contains every monomial symmetric function $P_{a_1,\dots,a_n}$ with $a_1 \geq d+1$, whose leading multiplicity is invertible in $\mathbb{F}$.*

The leading multiplicity of $P_{a_1,\dots,a_n}$ is, by definition, an integer between 1 and n. Theorem 5.1(a) is thus an immediate consequence of this lemma.

Proof. We will argue by induction on the weight r of $P_{a_1,\dots,a_n}$. For the base case, let $r = 1$. That is, we claim that $P_i \in J_{n,d}$ for every $i \geq d+1$. For $i = d+1, \dots, d+n$ this is given. Applying Newton's identities (cf., e.g., [7, pp. 23-24])

$$P_{m+n+1} = P_1 \cdot P_{m+n} - P_{1,1} \cdot P_{m+n-1} + \cdots + (-1)^{n+1} P_{\underbrace{1, \dots, 1}_{n \text{ times}}} \cdot P_{m+1}$$

recursively, with $m = d, d+1, d+2$, etc., we see that $P_{m+n+1} \in J_{n,d}$ for every $m \geq d$. This settles the base case.

For the induction step assume that $r \geq 2$. By (3),

$$P_{a_1} \cdot P_{a_2,\dots,a_r} = sP_{a_1,a_2,\dots,a_r} + P_{a_1+a_2,a_3,\dots,a_r} + P_{a_1+a_3,a_2,a_4,\dots,a_r} + \dots + P_{a_1+a_r,a_2,a_3,\dots,a_{r-1}}\,, \tag{5}$$

where s is the leading multiplicity of $P_{a_1,\dots,a_n}$. Each of the terms

$$P_{a_1+a_2,a_3,\dots,a_r},\ P_{a_1+a_3,a_2,a_4,\dots,a_r},\ \dots,\ P_{a_1+a_r,a_2,a_3,\dots,a_{r-1}}$$

is a monomial symmetric function of leading multiplicity 1 and weight $r-1$. By the induction assumption each of them lies in $J_{n,d}$. Since we also know that $P_{a_1} \in J_{n,d}$, equation (5) tells us that $P_{a_1,\dots,a_r} \in J_{n,d}$ whenever s is invertible in $\mathbb{F}$. □

We now turn to the proof of Theorem 5.1(b). Recall that it suffices to show that

$$P_{a_1,\dots,a_n} \in I \text{ whenever } a_1 \geq d+1. \tag{6}$$

Here I be the ideal of $R_n = \mathbb{F}[x_1, \dots, x_n]^{S_n}$ generated by the polynomials listed in the statement of Theorem 5.1(b). Denote the leading multiplicity of $P_{a_1,\dots,a_n}$ by s. We will now consider three cases.

Case 1. $s \neq p$. Since we are assuming that $n \leq 2p-1$, this is equivalent to s being invertible in $\mathbb{F}$. Clearly, $J_{n,d} \subset I$; Lemma 5.2 thus tells us that (6) holds.

Case 2. $s = p$ and $P_{a_1,\dots,a_n}$ has weight p. In other words, we want to show that

$$P_{\underbrace{a, \dots, a}_{p \text{ times}}} \in I\,. \tag{7}$$

Let $e = a - (d+1)$. By (3) we see that

$$P_{\underbrace{d+1, \dots, d+1}_{p \text{ times}}} \cdot P_{\underbrace{e, \dots, e}_{p \text{ times}}} = P_{\underbrace{a, \dots, a}_{p \text{ times}}} + \Gamma\,, \tag{8}$$

where Γ is a positive integer linear combination of monomial symmetric functions of leading multiplicity $\leq p-1$. Thus $\Gamma \in I$ by Case 1. Since by definition, $P_{\underbrace{d+1,\ldots,d+1}_{p \text{ times}}}$ lies in I, the left hand side also lies in I. This shows that (7) holds.

Note that the above argument depends, in a crucial way, on our assumption that $n \leq 2p-1$. For $n \geq 2p$ the sum Γ in (8) would contain a term of the form $P_{d+1,\ldots,d+1,e,\ldots,e}$ (or $P_{e,\ldots,e,d+1,\ldots,d+1}$, if $e > d+1$), with each e and $d+1$ repeating exactly p times. This monomial symmetric function has leading multiplicity p, and in the case we cannot conclude that $\Gamma \in I$.

Case 3. $s = p$, general case. Denote $a_1 = \cdots = a_p$ by a. Using formula (3) once again, we see that

$$P_{a_1,\ldots,a_n} = P_{\underbrace{a,\ldots,a}_{p \text{ times}}} \cdot P_{a_{p+1},\ldots,a_n} + \Delta\,,$$

where Δ is an integer linear combination of orbit sums $P_{c_1,\ldots,c_n}$ of leading multiplicity $\leq p-1$. Note that $P_{\underbrace{a,\ldots,a}_{p \text{ times}}} \in I$ by Case 2 and $\Delta \in I$ by Case 1. We thus conclude that $P_{a_1,\ldots,a_n} \in I$ as well. This completes the proof of Theorem 5.1. □

6. Regular sequences

We now turn to the question of whether or not the ideal $I_{n,d} = (x_1^{d+1},\ldots,x_n^{d+1}) \cap R_n$ of $R_n = \mathbb{F}[x_1,\ldots,x_n]^{\mathrm{S}_n}$ can be generated by a regular sequence. In the sequel we will sometimes use the same symbol for an element of R_n and its coset in $R_n/I_{n,d}$; we hope that this slight abuse of notation will make our formulas more transparent and will not lead to any confusion.

Our goal is to prove the following theorem.

Theorem 6.1. *Let $\mathbb{F}$ be a field of characteristic $p \geq 0$.*

(a) If $n!$ is not divisible by p then $I_{n,d}$ is generated by the regular sequence $P_{d+1},\ldots,P_{d+n}$ in R_n.

(b) Assume that $0 < p \leq n$ and either (i) $n \not\equiv -1$ (mod p) and $d \geq 1$ or (ii) $n \equiv -1$ (mod p) and $d \geq 2$. Then $I_{n,d}$ is not generated by any regular sequence in R_n.

The assumptions on d in part (b) cannot be dropped; see Remark 6.4. Our proof of Theorem 6.1 will rely on the following elementary lemma.

Lemma 6.2. *(a) The elements $P_{a_1,\ldots,a_n}$, with $d \geq a_1 \geq \cdots \geq a_n \geq 0$ form a basis for $R_n/I_{n,d}$ as an $\mathbb{F}$-vector space.*

(b) The Krull dimension of $R_n/I_{n,d}$ is 0.

(c) Suppose $I_{n,d}$ is generated by $r_1,\ldots,r_m \in R_n$, as an ideal of R_n. Then $m \geq n$. Moreover, $r_1,\ldots,r_m$ form a regular sequence in R_n if and only if $m = n$.

Proof. (a) The power sums $P_{a_1,\dots,a_n}$ with $a_1 \geq \cdots \geq a_n \geq 0$ form an $\mathbb{F}$-basis of R_n. The power sums $P_{a_1,\dots,a_n}$ with $a_1 \geq \cdots \geq a_n \geq 0$ and $a_1 \geq d+1$ form an $\mathbb{F}$-basis of $I_{n,d}$, and part (a) follows.
(b) By part (a) $R_n/I_{n,d}$ is a finite-dimensional $\mathbb{F}$-vector space.
(c) Recall that R_n is a polynomial ring over $\mathbb{F}$ generated by the elementary symmetric polynomials in $x_1, \dots, x_n$. In particular, R_n is a Cohen-Macauley ring. Part (c) now follows from part (b). □

Proof of Theorem 6.1. (a) If $p = \mathrm{char}(\mathbb{F})$ does not divide $n!$ then Theorem 5.1(a) tells us that $I_{n,d}$ is generated, as an ideal of R_n, by the n elements $P_{d+1}, \dots, P_{d+n}$. By Lemma 6.2(c) these elements form a regular sequence in R_n.
(b) If $I_{n,d}$ is generated by a regular sequence then $\mathrm{Socle}(R_n/I_{n,d})$ is a 1-dimensional $\mathbb{F}$-vector space; see, e.g. [9, p. 144] or [5, Section 21.2]. It is an immediate consequence of the multiplication formula (3) that

$$P_{\underbrace{d, \dots, d}_{n \text{ times}}} \in \mathrm{Socle}(R_n/I_{n,d})$$

for any $\mathbb{F}$, d and n.
Thus in order to show that $I_{n,d}$ is not generated by a regular sequence it suffices to exhibit a monomial symmetric function $P_{a_1,\dots,a_n} \in \mathrm{Socle}(R_n/I_{n,d})$, with $(a_1, \dots, a_n) \neq (d, \dots, d)$. Note that $P_{a_1,\dots,a_n}$ and $P_{\underbrace{d, \dots, d}_{n \text{ times}}}$ are $\mathbb{F}$-linearly independent in $R_n/I_{n,d}$ by Lemma 6.2(a).
(i) Suppose $d \geq 1$ and $n = pq + r$, where $q \geq 1$ and $r \in \{0, 1, \dots, p-2\}$. We claim that in this case $P_{a_1,\dots,a_n}$ lies in $\mathrm{Socle}(R_n/I_{n,d})$, if

$$a_1 = \cdots = a_{pq-1} = d \text{ and } a_{pq} = a_{pq+1} = \cdots = a_n = d - 1.$$

To establish this claim, we need to check that for these values of $a_1, \dots, a_n$,

$$P_{a_1,\dots,a_n} \cdot f \in I_{n,d}$$

for every $f \in R_n$. Since R_n is generated by the elementary symmetric polynomials P_1, $P_{1,1}$, etc., it suffices to show that

$$P_{a_1,\dots,a_n} \cdot P_{b_1,\dots,b_n} \in I_{n,d}, \tag{9}$$

where

$$(b_1, \dots, b_n) = (\underbrace{1, \dots, 1}_{s \text{ times}}, 0, \dots, 0)\,. \tag{10}$$

We want to prove (9) for each $s = 1, \dots, n$.
Let us examine the product $P_{a_1,\dots,a_n} \cdot P_{b_1,\dots,b_n}$ using the multiplication formula (3). First of all, note that we may assume without loss of generality that $1 \leq s \leq r+1$. Indeed, if $s > r+1$ then every term $P_{c_1,\dots,c_n}$ appearing in the right hand side of the formula (3) will have $c_1 \geq d+1$ and thus will lie in $I_{n,d}$ (for any base field $\mathbb{F}$).

If $1 \leq s \leq r+1$, the only monomial symmetric functions $P_{c_1,\dots,c_n}$, with $c_1 \leq d$, appearing in the right hand side of (3), will have $c_1 = \cdots = c_{pq+s-1} = d$ and $c_{pq+s} = c_{pq+s+1} = \cdots = c_n = d-1$. This sum will appear with coefficient $k_{c_1,\dots,c_n}$ = number of ways to write $(c_1,\dots,c_n)$ as $(a'_1,\dots,a'_n) + (b'_1,\dots,b'_n)$, where $(a'_1,\dots,a'_n)$ is a permutation of $(a_1,\dots,a_n)$ and $(b'_1,\dots,b'_n)$ is a permutation of $(b_1,\dots,b_n)$. We claim that $k_{c_1,\dots,c_n}$ is divisible by p and hence, is 0 in $\mathbb{F}$; this will immediately imply (9). Indeed, in this case $k_{c_1,\dots,c_n}$ is simply the number of ways to specify which s of the elements $b'_1,\dots,b'_{pq+s-1}$ should be equal to 1 (the remaining ones will be 0). Thus

$$k_{c_1,\dots,c_n} = \binom{pq+s-1}{s}.$$

Since $q \geq 1$ and $1 \leq s \leq r+1 \leq p-1$, this number is divisible by p, as claimed.

(ii) Now suppose $d \geq 2$ and $n = pq+p-1$, where $q \geq 1$. We claim that in this case $P_{a_1,\dots,a_n}$ lies in $\mathrm{Socle}(R_n/I_{n,d})$, if

$$a_1 = \cdots = a_{pq-1} = d,\ a_{pq} = a_{pq+1} = \cdots = a_{pq+p-2} = d-1$$

and $a_{pq+p-1} = d-2$. Once again, it suffices to show that (9) holds for every $s = 1,\dots,n$, where $(b_1,\dots,b_n)$ is as in (10). The analysis of the product $P_{a_1,\dots,a_n} \cdot P_{b_1,\dots,b_n}$, based on formula (3), is similar to part (i) but a bit more involved.

First of all, we may assume without loss of generality that $1 \leq s \leq p$. Indeed, if $s \geq p+1$, then every monomial symmetric function $P_{c_1,\dots,c_n}$ appearing in the right hand side of (3) will lie in $I_{n,d}$, so that (9) will hold over any base field $\mathbb{F}$.

If $1 \leq s \leq p$ then only two monomial symmetric functions $P_{c_1,\dots,c_n}$ with $c_1 \leq d$ will appear in the right hand side of (3), namely

$$P_{\underbrace{d,\dots,d}_{pq+s-2},\ \underbrace{d-1,\dots,d-1}_{p-s+1}}$$

and

$$P_{\underbrace{d,\dots,d}_{pq+s-1},\ \underbrace{d-1,\dots,d-1}_{p-s-1},\ d-2}$$

with coefficients

$$k_{\underbrace{d,\dots,d}_{pq+s-2},\ \underbrace{d-1,\dots,d-1}_{p-s+1}} = \binom{pq+s-2}{s-1}(p-s+1)$$

and

$$k_{\underbrace{d,\dots,d}_{pq+s-1},\ \underbrace{d-1,\dots,d-1}_{p-s-1},\ d-2} = \binom{pq+s-1}{s},$$

respectively. (The second monomial symmetric function does not occur if $s = p$.) Both of these coefficients are divisible by p and hence, are 0 in $\mathbb{F}$. This completes the proof of Theorem 6.1. □

Corollary 6.3. *Suppose (i) $p \leq n \leq 2p-2$ and $d \geq 1$ or (ii) $n = 2p-1$ and $d \geq 2$. Then the ideal $I_{n,d}$ can be generated by $n+1$ elements of R_n but cannot be generated by n elements.*

Proof. Theorem 5.1(b) tells us that $I_{n,d}$ is generated by $n+1$ elements. If $I_{n,d}$ could be generated by n elements then by Lemma 6.2(c) these n elements would form a regular sequence in R_n, contradicting Theorem 6.1(b). □

Remark 6.4. The conditions that $d \geq 1$ and $d \geq 2$ in parts (i) and (ii) of Theorem 6.1(b) respectively, cannot be dropped. The same goes for conditions (i) and (ii) in Corollary 6.3.
Indeed, suppose $d = 0$. Recall that $R_n = \mathbb{F}[x_1, \ldots, x_n]^{S_n}$ is a polynomial algebra $\mathbb{F}[s_1, \ldots, s_n]$, where $s_1 = P_1$, $s_2 = P_{1,1}$, etc., are the elementary symmetric polynomials in $x_1, \ldots, x_n$. $I_{n,0}$ is clearly the maximal ideal of R_n generated by the regular sequence $s_1, \ldots, s_n$. Thus Theorem 6.1(b) fails if $d = 0$.
Now suppose $d = 1$ and $n = 2p-1$, where $\mathrm{char}(\mathbb{F}) = p$. By Theorem 5.1(b), $I_{n,1}$ is generated by the $n+1$ elements $P_2, \ldots, P_{n-1}, P_{n+1}$ and $P_{\underbrace{2,\ldots,2}_{p \text{ times}}}$.
Since we are in characteristic p, $P_{n+1} = P_{2p} = P_2^p$, is a redundant generator. In other words, $I_{n,1}$ is generated by the n elements $P_2, \ldots, P_{n-1}, P_n$ and $P_{\underbrace{2,\ldots,2}_{p \text{ times}}}$.
By Lemma 6.2(c) these elements form a regular sequence in R_n. This shows that Theorem 6.1(b) fails for $d = 1$ and $n = 2p-1$. □

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A Lefschetz Fixed Point Formula for Singular Arithmetic Schemes with Smooth Generic Fibres

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Abstract. In this article, we consider singular equivariant arithmetic schemes whose generic fibres are smooth. For such schemes, we prove a relative fixed point formula of Lefschetz type in the context of Arakelov geometry. This formula is an analog, in the arithmetic case, of the Lefschetz formula proved by R. W. Thomason in [31]. In particular, our result implies a fixed point formula which was conjectured by V. Maillot and D. Rössler in [25].

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1 Introduction

It is the aim of this article to prove a singular Lefschetz fixed point formula for some schemes which admit the actions of a diagonalisable group scheme, in the context of Arakelov geometry. We first roughly describe the history of the study of such Lefschetz fixed point formulae and relative Lefschetz-Riemann-Roch problems.

Let k be an algebraically closed field and let n be an integer which is prime to the characteristic of k. A projective $k-$variety X which admits an automorphism g of order n will be called an equivariant variety. An equivariant coherent sheaf on X is a coherent sheaf F on X together with a homomorphism $\varphi : g^*F \to F$. It is clear that this homomorphism induces a family of endomorphisms $H^i(\varphi)$ on cohomology spaces $H^i(X, F)$.

A classical Lefschetz fixed point formula is to give an expression of the alternating sum of the traces of $H^i(\varphi)$, as a sum of the contributions from the components of the fixed point subvariety X_g. On the other hand, roughly speaking, a Lefschetz-Riemann-Roch theorem is a commutative diagram in equivariant $K-$theory which can be regarded as a Grothendieck type generalization of the Lefschetz fixed point formula. Indeed, when we choose the base variety in such a commutative diagram to be a point, we will get the ordinary Lefschetz fixed point formula. If X is nonsingular, P. Donovan has proved such a theorem in [12] by using the results and some of the methods of the paper of A. Borel and J. P. Serre on the Grothendieck-Riemann-Roch theorem (cf. [10]). In [1], P. Baum, W. Fulton and G. Quart generalized Donovan's theorem to singular varieties, the key step of their proof heavily relies on an elegant method called the deformation to the normal cone. Denote by $G_0(X,g)$ (resp. $K_0(X,g)$) the Quillen's algebraic K-group associated to the category of equivariant coherent sheaves (resp. vector bundles of finite rank) on X, then $K_0(\mathrm{Pt},g)$ is isomorphic to the group ring $\mathbb{Z}[k]$ and $G_0(X,g)$ (resp. $K_0(X,g)$) has a natural $K_0(\mathrm{Pt},g)$-module (resp. $K_0(\mathrm{Pt},g)$-algebra) structure. Let f be an equivariantly projective morphism between two equivariant varieties X and Y, then it is possible to define a push-forward morphism f_* from $G_0(X,g)$ to $G_0(Y,g)$ in a rather standard way. Let $\mathcal{R}$ be any flat $K_0(\mathrm{Pt},g)$-algebra in which $1-\zeta$ is invertible for each non-trivial n-th root of unity ζ in k. The main result of Baum, Fulton and Quart reads: there exists a family of group homomorphisms $L.$ between K-groups making the following diagram

$$\begin{array}{ccc} G_0(X,g) & \xrightarrow{L.} & G_0(X_g,g)\otimes_{\mathbb{Z}[k]}\mathcal{R} \\ \downarrow{\scriptstyle f_*} & & \downarrow{\scriptstyle f_{g*}} \\ G_0(Y,g) & \xrightarrow{L.} & G_0(Y_g,g)\otimes_{\mathbb{Z}[k]}\mathcal{R} \end{array}$$

commutative. If Z is a nonsingular equivariant variety such that there exists an equivariant closed immersion from X to Z, then for every equivariant coherent sheaf E on X the homomorphism $L.$ is exactly given by the formula

$$L.(E)=\lambda_{-1}^{-1}(N_{Z/Z_g}^\vee)\cdot\sum_j(-1)^j\mathrm{Tor}^j_{\mathcal{O}_Z}(i_*E,\mathcal{O}_{Z_g})$$

where N_{Z/Z_g} stands for the normal bundle of Z_g in Z and $\lambda_{-1}(N_{Z/Z_g}^\vee):=\sum(-1)^j\wedge^j N_{Z/Z_g}^\vee$.

We would like to indicate that one can use the same method so called the deformation to the normal cone to extend Baum, Fulton and Quart's result to general scheme case where X and Y are Noetherian, separated schemes endowed with projective actions of the diagonalisable group scheme μ_n associated to $\mathbb{Z}/n\mathbb{Z}$. Here by a μ_n-action on X we understand a morphism $m_X:\mu_n\times X\to X$ which statisfies some compatibility properties. Denote by p_X the projection from $\mu_n\times X$ to X. For a coherent $\mathcal{O}_X$-module E on X, a μ_n-action on E we mean an isomorphism $m_E : p_X^*E \to m_X^*E$ which satisfies certain associativity properties. We refer to [20] and [21, Section 2] for the group scheme action theory we are talking about.

In [31], R. W. Thomason used another way to generalize Baum, Fulton and Quart's result to the scheme case, and he removed the condition of projectivity. The strategy Thomason followed was to use Quillen's localization sequence for higher equivariant K-groups to prove an algebraic concentration theorem. Let D be an integral Noetherian ring, and let μ_n be the diagonalisable group scheme over D associated to $\mathbb{Z}/n\mathbb{Z}$. Denote the ring $K_0(D,\mu_n) \cong K_0(D)[T]/(1-T^n)$ by $R(\mu_n)$. We consider the prime ideal ρ in $R(\mu_n)$ with which the intersection of $\mathbb{Z}[\mathbb{Z}/n\mathbb{Z}]$ is exactly the kernel of the canonical morphism $\mathbb{Z}[T]/(1-T^n) \to \mathbb{Z}[T]/(\Phi_n)$ where Φ_n stands for the n-th cyclotomic polynomial (cf. [31, Lem. 1.6]). By construction the elements $1-T^k$ for $k=1,\ldots,n-1$ are not contained in ρ. Let X be a μ_n-equivariant scheme over D, then $G_0(X,\mu_n)$ (resp. $K_0(X,\mu_n)$) has a natural $R(\mu_n)$-module (resp. $R(\mu_n)$-algebra) structure. Denote by i the inclusion from X_{μ_n} to X. The algebraic concentration theorem reads: there exists a natural group homomorphism i_* from $G_0(X_{\mu_n},\mu_n)_\rho$ to $G_0(X,\mu_n)_\rho$ which is an isomorphism. Moreover, if X is regular, the inverse map of i_* is given by $\lambda_{-1}^{-1}(N_{X/X_{\mu_n}}^\vee)\cdot i^*$ where $N_{X/X_{\mu_n}}$ is the normal bundle of X_{μ_n} in X. This concentration theorem can be used to prove a singular Lefschetz fixed point formula which is an extension of Baum, Fulton and Quart's result in general scheme case. Thomason's approach has nothing to do with the construction of the deformation to the normal cone, and the localization he used is slightly weaker than Baum, Fulton and Quart's in the sense that the complement of the ideal ρ in $R(\mu_n)$ is not the smallest algebra in which the elements $1-T^k$ $(k=1,\ldots,n-1)$ are invertible. If one exactly chooses $\mathcal{R}$ to be the complement of the ideal ρ in $R(\mu_n)$, then these two localizations are equal to each other.

In [21], K. Köhler and D. Rössler generalized the regular case of Baum, Fulton and Quart's result to Arakelov geometry. To every regular μ_n-equivariant arithmetic scheme X, they associate an equivariant arithmetic K_0-group $\widehat{K_0}(X,\mu_n)$ which contains some smooth form class on $X_{\mu_n}(\mathbb{C})$ as analytic datum. Such an equivariant arithmetic K_0-group has a ring structure so that it is also an $R(\mu_n)$-algebra. Let $\overline{N}_{X/X_{\mu_n}}$ be the normal bundle with respect to the regular immersion $X_{\mu_n} \hookrightarrow X$ which is endowed with the quotient metric induced by a chosen Kähler metric of $X(\mathbb{C})$, then the main theorem in [21] reads: the element $\lambda_{-1}(\overline{N}_{X/X_{\mu_n}}^\vee)$ is invertible in $\widehat{K_0}(X_{\mu_n},\mu_n)\otimes_{R(\mu_n)}\mathcal{R}$ and we have the following commutative diagram

$$\begin{array}{ccc}
\widehat{K_0}(X,\mu_n) & \xrightarrow{\Lambda_R(f)^{-1}\cdot\tau} & \widehat{K_0}(X_{\mu_n},\mu_n)\otimes_{R(\mu_n)}\mathcal{R} \\
\downarrow{\scriptstyle f_*} & & \downarrow{\scriptstyle f_{\mu_n *}} \\
\widehat{K_0}(D,\mu_n) & \xrightarrow{\iota} & \widehat{K_0}(D,\mu_n)\otimes_{R(\mu_n)}\mathcal{R}
\end{array}$$

where $\Lambda_R(f) := \lambda_{-1}(\overline{N}^{\vee}_{X/X_{\mu_n}}) \cdot (1 + R_g(N_{X/X_{\mu_n}}))$, τ stands for the restriction map and ι is the natural morphism from a ring or a module to its localization which sends an element e to $\frac{e}{1}$. Here $R_g(\cdot)$ is the equivariant R-genus, the definition of the two push-forward morphisms f_* and $f_{\mu_n *}$ involves an important analytic datum which is called the equivariant analytic torsion. The strategy Köhler and Rössler followed to prove such an arithmetic Lefschetz-Riemann-Roch theorem was to use the construction of the deformation to the normal cone to prove an analog of this theorem for equivariant closed immersions. After that, they decompose the morphism f to a closed immersion h from X to some projective space $\mathbb{P}^r_D$ followed by a smooth morphism p from $\mathbb{P}^r_D$ to $\mathrm{Spec}(D)$. Then the theorem in general situation follows from an argument of investigating the behavior of the error term under the morphisms h and p.

Provided X. Ma's extension of equivariant analytic torsion to higher equivariant analytic torsion form, it was conjectured by Köhler and Rössler in [22] that an analog of [21, Theorem 4.4] in relative setting holds. We have already proved this conjecture in [29]. Our method is similar to Thomason's, we first show that there exists an arithmetic concentration theorem in Arakelov geometry and then deduce from it the relative Lefschetz fixed point formula. The same as Thomason's approach, our method has nothing to do with the construction of the deformation to the normal cone, but unfortunately it only works for regular arithmetic schemes.

One may naturally asked that whether it is possible to construct a more general arithmetic $\widehat{G_0}$-theory and prove a relative Lefschetz fixed point formula for singular arithmetic schemes which is entirely an analog of Thomason's singular Lefschetz formula in Arakelov geometry. The answer is Yes, and this is what we have done in this article. To do this, one needs a $\widehat{G_0}$-theoretic vanishing theorem which can be viewed as an extension of Köhler and Rössler's fixed point formula for closed immersions to the singular case. The proof of such a vanishing theorem occupies a lot of space in this article. Let X and Y be two singular equivariant arithmetic schemes with smooth generic fibres, and let $f: X \to Y$ be an equivariant morphism which is smooth on the complex numbers. Assume that the μ_n-action on Y is trivial and f can be decomposed to be $h \circ i$ where i is an equivariant closed immersion from X to some regular arithmetic scheme Z and $h: Z \to Y$ is equivariant and smooth on the complex numbers. Let $\overline{\eta}$ be an equivariant hermitian sheaf on X. Referring to Section 6.1 for the explanations of various notations, we announce that our main theorem in this article is the following equality which holds in $\widehat{G_0}(Y, \mu_n, \emptyset)_\rho$:

$$\begin{aligned} f_*(\overline{\eta}) =& f^Z_{\mu_n *}(i^*_{\mu_n}(\lambda^{-1}_{-1}(\overline{N}^{\vee}_{Z/Z_{\mu_n}})) \cdot \sum_k (-1)^k \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}})) \\ &+ \int_{X_g/Y} \mathrm{Td}(Tf_g, \omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}}, \omega^X)\mathrm{Td}^{-1}_g(\overline{F}) \\ &- \int_{X_g/Y} \mathrm{Td}_g(Tf)\mathrm{ch}_g(\eta)R_g(N_{X/X_g}) \end{aligned}$$

$$+\int_{X_g/Y}\widetilde{\mathrm{Td}}(Tf_g,\omega^X,\omega^Z_X)\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\mathrm{Td}_g^{-1}(\overline{F}).$$

The structure of this article is as follows. In Section 2, we recall some differential-geometric facts for the convenience of the reader. In Section 3, we formulate and prove a vanishing theorem for equivariant closed immersions in a purely analytic setting. In Section 4, we define the arithmtic G_0-groups with respect to fixed wave front sets which are necessary for our later arguments. In Section 5 and Section 6, we formulate and prove the arithmetic concentration theorem and the relative Lefschetz fixed point formula for singular arithmetic schemes.

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2 Differential-geometric preliminaries

2.1 Equivariant Chern-Weil theory

Let G be a compact Lie group and let M be a compact complex manifold which admits a holomorphic G-action. By an equivariant hermitian vector bundle on M, we understand a hermitian vector bundle on M which admits a G-action compatible with the G-structure of M and whose metric is G-invariant. Let $g\in G$ be an automorphism of M, we shall denote by $M_g=\{x\in M\mid g\cdot x=x\}$ the fixed point submanifold. M_g is also a compact complex manifold.
Now let $\overline{E}$ be an equivariant hermitian vector bundle on M, it is well known that the restriction of $\overline{E}$ to M_g splits as a direct sum

$$\overline{E}\mid_{M_g}=\bigoplus_{\zeta\in S^1}\overline{E}_\zeta$$

where the equivariant structure g^E of E acts on $\overline{E}_\zeta$ as multiplication by ζ. We often write $\overline{E}_g$ for $\overline{E}_1$ and call it the 0-degree part of $\overline{E}\mid_{M_g}$. As usual, $A^{p,q}(M)$ stands for the space of (p,q)-forms $\Gamma^\infty(M,\Lambda^pT^{*(1,0)}M\wedge\Lambda^qT^{*(0,1)}M)$, we define

$$\widetilde{A}(M)=\bigoplus_{p=0}^{\dim M}(A^{p,p}(M)/(\mathrm{Im}\partial+\mathrm{Im}\overline{\partial})).$$

We denote by $\Omega^{\overline{E}_\zeta}\in A^{1,1}(M_g)$ the curvature form associated to $\overline{E}_\zeta$. Let $(\phi_\zeta)_{\zeta\in S^1}$ be a family of $\mathbf{GL}(\mathbb{C})$-invariant formal power series such that $\phi_\zeta\in\mathbb{C}[[\mathbf{gl}_{\mathrm{rk}E_\zeta}(\mathbb{C})]]$ where $\mathrm{rk}E_\zeta$ stands for the rank of E_ζ which is a locally constant function on M_g. Moreover, let $\phi\in\mathbb{C}[[\bigoplus_{\zeta\in S^1}\mathbb{C}]]$ be any formal power series. We have the following definition.

DEFINITION 2.1. The way to associate a smooth form to an equivariant hermitian vector bundle $\overline{E}$ by setting

$$\phi_g(\overline{E}) := \phi((\phi_\zeta(-\frac{\Omega^{\overline{E}_\zeta}}{2\pi i}))_{\zeta\in S^1})$$

is called an g-equivariant Chern-Weil theory associated to $(\phi_\zeta)_{\zeta\in S^1}$ and ϕ. The class of $\phi_g(\overline{E})$ in $\widetilde{A}(M_g)$ is independent of the metric.

Write dd^c for the differential operator $\frac{\overline{\partial}\partial}{2\pi i}$. The theory of equivariant secondary characteristic classes is described in the following theorem.

THEOREM 2.2. *To every short exact sequence* $\overline{\varepsilon} : 0 \to \overline{E}' \to \overline{E} \to \overline{E}'' \to 0$ *of equivariant hermitian vector bundles on* M*, there is a unique way to attach a class* $\widetilde{\phi}_g(\overline{\varepsilon}) \in \widetilde{A}(M_g)$ *which satisfies the following three conditions:*
(i). $\widetilde{\phi}_g(\overline{\varepsilon})$ *satisfies the differential equation*

$$\mathrm{dd}^c\widetilde{\phi}_g(\overline{\varepsilon}) = \phi_g(\overline{E}' \oplus \overline{E}'') - \phi_g(\overline{E});$$

(ii). for every equivariant holomorphic map $f : M' \to M$*,* $\widetilde{\phi}_g(f^*\overline{\varepsilon}) = f_g^*\widetilde{\phi}_g(\overline{\varepsilon})$*;*
(iii). $\widetilde{\phi}_g(\overline{\varepsilon}) = 0$ *if* $\overline{\varepsilon}$ *is equivariantly and orthogonally split.*

Proof. This is [21, Theorem 3.4]. □

We now give some examples of equivariant character forms and their corresponding secondary characteristic classes.

EXAMPLE 2.3. (i). The equivariant Chern character form $\mathrm{ch}_g(\overline{E}) := \sum_{\zeta\in S^1}\zeta\mathrm{ch}(\overline{E}_\zeta)$.
(ii). The equivariant Todd form $\mathrm{Td}_g(\overline{E}) := \frac{c_{\mathrm{rk}E_g}(\overline{E}_g)}{\mathrm{ch}_g(\sum_{j=0}^{\mathrm{rk}E}(-1)^j\wedge^j\overline{E}^\vee)}$. As in [18, Thm. 10.1.1] one can show that

$$\mathrm{Td}_g(\overline{E}) = \mathrm{Td}(\overline{E}_g)\prod_{\zeta\neq 1}\det(\frac{1}{1-\zeta^{-1}e^{\frac{\Omega^{\overline{E}_\zeta}}{2\pi i}}}).$$

(iii). Let $\overline{\varepsilon} : 0 \to \overline{E}' \to \overline{E} \to \overline{E}'' \to 0$ be a short exact sequence of hermitian vector bundles. The secondary Bott-Chern characteristic class is given by $\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}) = \sum_{\zeta\in S^1}\zeta\widetilde{\mathrm{ch}}(\overline{\varepsilon}_\zeta)$.
(iv). If the equivariant structure g^ε has the eigenvalues $\zeta_1, \cdots, \zeta_m$, then the secondary Todd class is given by

$$\widetilde{\mathrm{Td}}_g(\overline{\varepsilon}) = \sum_{i=1}^m\prod_{j=1}^{i-1}\mathrm{Td}_g(\overline{E}_{\zeta_j})\cdot\widetilde{\mathrm{Td}}(\overline{\varepsilon}_{\zeta_i})\cdot\prod_{j=i+1}^m\mathrm{Td}_g(\overline{E}'_{\zeta_j}+\overline{E}''_{\zeta_j}).$$

REMARK 2.4. One can use Theorem 2.2 to give a proof of the statements (iii) and (iv) in the examples above.

Let E be an equivariant hermitian vector bundle with two different hermitian metrics h_1 and h_2, we shall write $\widetilde{\phi}_g(E,h_1,h_2)$ for the equivariant secondary characteristic class associated to the exact sequence

$$0 \to (E,h_1) \to (E,h_2) \to 0 \to 0$$

where the map from (E,h_1) to (E,h_2) is the identity map.

2.2 Equivariant analytic torsion forms

In [7], J.-M. Bismut and K. Köhler extended the Ray-Singer analytic torsion to the higher analytic torsion form T for a holomorphic submersion. The purpose of making such an extension is that the differential equation on dd^cT gives a refinement of the Grothendieck-Riemann-Roch theorem. Later, in his article [23], X. Ma generalized J.-M. Bismut and K. Köhler's results to the equivariant case. In this subsection, we shall briefly recall Ma's construction of the equivariant analytic torsion form. This construction is not very important for understanding the rest of this article, but the equivariant analytic torsion form itself will be used to define a reasonable push-forward morphism between equivariant arithmetic G_0-groups.

We first fix some notations and assumptions. Let $f: M \to B$ be a proper holomorphic submersion of complex manifolds, and let TM, TB be the holomorphic tangent bundle on M, B. Denote by J^{Tf} the complex structure on the real relative tangent bundle $T_{\mathbb{R}}f$, and assume that h^{Tf} is a hermitian metric on Tf which induces a Riemannian metric g^{Tf}. Let T^HM be a vector subbundle of TM such that $TM = T^HM \oplus Tf$, the following definition of Kähler fibration was given in [4, Def. 1.4].

Definition 2.5. The triple (f, h^{Tf}, T^HM) is said to define a Kähler fibration if there exists a smooth real $(1,1)-$form ω which satisfies the following three conditions:

(i). ω is closed;

(ii). $T_{\mathbb{R}}^HM$ and $T_{\mathbb{R}}f$ are orthogonal with respect to ω;

(iii). if $X, Y \in T_{\mathbb{R}}f$, then $\omega(X,Y) = \langle X, J^{Tf}Y\rangle_{g^{Tf}}$.

It was shown in [4, Thm. 1.5 and 1.7] that for a given Kähler fibration, the form ω is unique up to addition of a form $f^*\eta$ where η is a real, closed $(1,1)$-form on B. Moreover, for any real, closed $(1,1)$-form ω on M such that the bilinear map $X, Y \in T_{\mathbb{R}}f \mapsto \omega(J^{Tf}X, Y) \in \mathbb{R}$ defines a Riemannian metric and hence a hermitian product h^{Tf} on Tf, we can define a Kähler fibration whose associated $(1,1)$-form is ω. In particular, for a given f, a Kähler metric on M defines a Kähler fibration if we choose T^HM to be the orthogonal complement of Tf in TM and ω to be the Kähler form associated to this metric.

We now recall the Bismut superconnection of a Kähler fibration. Let (ξ, h^ξ) be a hermitian complex vector bundle on M. Let ∇^{Tf}, ∇^ξ be the holomorphic hermitian connections on (Tf, h^{Tf}) and (ξ, h^{ξ}). Let $\nabla^{\Lambda(T^{*(0,1)}f)}$ be the connection induced by ∇^{Tf} on $\Lambda(T^{*(0,1)}f)$. Then we may define a connection on $\Lambda(T^{*(0,1)}f)\otimes\xi$ by setting

$$\nabla^{\Lambda(T^{*(0,1)}f)\otimes\xi}=\nabla^{\Lambda(T^{*(0,1)}f)}\otimes 1+1\otimes\nabla^{\xi}.$$

Let E be the infinite-dimensional bundle on B whose fibre at each point $b\in B$ consists of the C^∞ sections of $\Lambda(T^{*(0,1)}f)\otimes\xi\mid_{f^{-1}b}$. This bundle E is a smooth $\mathbb{Z}$-graded bundle. We define a connection ∇^E on E as follows. If $U\in T_{\mathbb{R}}B$, let U^H be the lift of U in $T^H_{\mathbb{R}}M$ so that $f_*U^H=U$. Then for every smooth section s of E over B, we set

$$\nabla^E_U s=\nabla^{\Lambda(T^{*(0,1)}f)\otimes\xi}_{U^H}s.$$

For $b\in B$, let $\overline{\partial}^{Z_b}$ be the Dolbeault operator acting on E_b, and let $\overline{\partial}^{Z_b*}$ be its formal adjoint with respect to the canonical hermitian product on E_b (cf. [23, 1.2]). Let $C(T_{\mathbb{R}}f)$ be the Clifford algebra of $(T_{\mathbb{R}}f, h^{Tf})$, then the bundle $\Lambda(T^{*(0,1)}f)\otimes\xi$ has a natural $C(T_{\mathbb{R}}f)$-Clifford module structure. Actually, if $U\in Tf$, let $U'\in T^{*(0,1)}f$ correspond to U defined by $U'(\cdot)=h^{Tf}(U,\cdot)$, then for $U,V\in Tf$ we set

$$c(U)=\sqrt{2}U'\wedge,\quad c(\overline{V})=-\sqrt{2}i_{\overline{V}}$$

where $i_{(\cdot)}$ is the contraction operator (cf. [9, Definition 1.6]). Moreover, if $U,V\in T_{\mathbb{R}}B$, we set $T(U^H,V^H)=-P^{Tf}[U^H,V^H]$ where P^{Tf} stands for the canonical projection from TM to Tf.

Definition 2.6. Let $e_1,\dots,e_{2m}$ be a basis of $T_{\mathbb{R}}B$, and let $e^1,\dots,e^{2m}$ be the dual basis of $T^*_{\mathbb{R}}B$. Then the element

$$c(T)=\frac{1}{2}\sum_{1\leq\alpha,\beta\leq 2m}e^\alpha\wedge e^\beta\widehat{\otimes}c(T(e^H_\alpha,e^H_\beta))$$

is a section of $(f^*\Lambda(T^*_{\mathbb{R}}B)\widehat{\otimes}\mathrm{End}(\Lambda(T^{*(0,1)}f)\otimes\xi))^{\mathrm{odd}}$.

Definition 2.7. For $u>0$, the Bismut superconnection on E is the differential operator

$$B_u=\nabla^E+\sqrt{u}(\overline{\partial}^Z+\overline{\partial}^{Z*})-\frac{1}{2\sqrt{2u}}c(T)$$

on $f^*(\Lambda(T^*_{\mathbb{R}}B))\widehat{\otimes}(\Lambda(T^{*(0,1)}f)\otimes\xi)$.

Definition 2.8. Let N_V be the number operator on $\Lambda(T^{*(0,1)}f)\otimes\xi$ and on E, namely N_V acts as multiplication by p on $\Lambda^p(T^{*(0,1)}f)\otimes\xi$. For $U,V\in T_{\mathbb{R}}B$, set $\omega^{H\overline{H}}(U,V)=\omega^M(U^H,V^H)$ where ω^M is the closed form in the definition of Kähler fibration. Furthermore, for $u>0$, set $N_u=N_V+\frac{i\omega^{H\overline{H}}}{u}$.

We now turn to the equivariant case. Let G be a compact Lie group, we shall assume that all complex manifolds, hermitian vector bundles and holomorphic morphisms considered above are $G-$equivariant and all metrics are G-invariant. We will additionally assume that the direct images $R^k f_*\xi$ are all locally free so that the G-equivariant coherent sheaf $R^\cdot f_*\xi$ is locally free and hence a G-equivariant vector bundle over B. [23, 1.2] gives a G-invariant hermitian metric (the L^2-metric) $h^{R^\cdot f_*\xi}$ on the vector bundle $R^\cdot f_*\xi$.
For $g\in G$, let $M_g=\{x\in M\mid g\cdot x=x\}$ and $B_g=\{b\in B\mid g\cdot b=b\}$ be the fixed point submanifolds, then f induces a holomorphic submersion $f_g: M_g\to B_g$. Let Φ be the homomorphism $\alpha\mapsto (2i\pi)^{-\deg\alpha/2}$ of $\Lambda^{\rm even}(T^*_{\mathbb{R}}B)$ into itself. We put

$$\mathrm{ch}_g(R^\cdot f_*\xi,h^{R^\cdot f_*\xi})=\sum_{k=0}^{\dim M-\dim B}(-1)^k\mathrm{ch}_g(R^kf_*\xi,h^{R^kf_*\xi})$$

and

$$\mathrm{ch}'_g(R^\cdot f_*\xi,h^{R^\cdot f_*\xi})=\sum_{k=0}^{\dim M-\dim B}(-1)^k k\,\mathrm{ch}_g(R^kf_*\xi,h^{R^kf_*\xi}).$$

Definition 2.9. For $s\in\mathbb{C}$ with $\mathrm{Re}(s)>1$, let

$$\zeta_1(s)=-\frac{1}{\Gamma(s)}\int_0^1 u^{s-1}(\Phi\mathrm{Tr_s}[gN_u\exp(-B_u^2)]-\mathrm{ch}'_g(R^\cdot f_*\xi,h^{R^\cdot f_*\xi}))\mathrm{d}u$$

and similarly for $s\in\mathbb{C}$ with $\mathrm{Re}(s)<\frac{1}{2}$, let

$$\zeta_2(s)=-\frac{1}{\Gamma(s)}\int_1^\infty u^{s-1}(\Phi\mathrm{Tr_s}[gN_u\exp(-B_u^2)]-\mathrm{ch}'_g(R^\cdot f_*\xi,h^{R^\cdot f_*\xi}))\mathrm{d}u.$$

X. Ma has proved that $\zeta_1(s)$ extends to a holomorphic function of $s\in\mathbb{C}$ near $s=0$ and $\zeta_2(s)$ is a holomorphic function of s.

Definition 2.10. The smooth form $T_g(\omega^M,h^\xi):=\frac{\partial}{\partial s}(\zeta_1+\zeta_2)(0)$ on B_g is called the equivariant analytic torsion form.

Theorem 2.11. *The form $T_g(\omega^M,h^\xi)$ lies in $\bigoplus_{p\geq 0}A^{p,p}(B_g)$ and satisfies the following differential equation*

$$\mathrm{dd}^cT_g(\omega^M,h^\xi)=\mathrm{ch}_g(R^\cdot f_*\xi,h^{R^\cdot f_*\xi})-\int_{M_g/B_g}\mathrm{Td}_g(Tf,h^{Tf})\mathrm{ch}_g(\xi,h^\xi).$$

Here $A^{p,p}(B_g)$ stands for the space of smooth forms on B_g of type (p,p).

Proof. This is [23, Theorem 2.12]. □

We define a secondary characteristic class

$$\widetilde{\mathrm{ch}}_g(R^\cdot f_*\xi,h^{R^\cdot f_*\xi},h'^{R^\cdot f_*\xi}):=\sum_{k=0}^{\dim M-\dim B}(-1)^k\widetilde{\mathrm{ch}}_g(R^kf_*\xi,h^{R^kf_*\xi},h'^{R^kf_*\xi})$$

such that it satisfies the following differential equation

$$\mathrm{dd}^c\widetilde{\mathrm{ch}}_g(R^\cdot f_*\xi, h^{R^\cdot f_*\xi}, h'^{R^\cdot f_*\xi}) = \mathrm{ch}_g(R^\cdot f_*\xi, h^{R^\cdot f_*\xi}) - \mathrm{ch}_g(R^\cdot f_*\xi, h'^{R^\cdot f_*\xi}),$$

then the anomaly formula can be described as follows.

THEOREM 2.12. *(Anomaly formula) Let ω' be the form associated to another Kähler fibration for $f: M \to B$. Let h'^{Tf} be the metric on Tf in this new fibration and let h'^{ξ} be another metric on ξ. The following identity holds in $\widetilde{A}(B_g) := \bigoplus_{p\geq 0}(A^{p,p}(B_g)/(\mathrm{Im}\partial + \mathrm{Im}\overline{\partial}))$:*

$$\begin{aligned} T_g(\omega^M, h^\xi) - T_g(\omega'^M, h'^\xi) =& \widetilde{\mathrm{ch}}_g(R^\cdot f_*\xi, h^{R^\cdot f_*\xi}, h'^{R^\cdot f_*\xi}) \\ & - \int_{M_g/B_g} [\widetilde{\mathrm{Td}}_g(Tf, h^{Tf}, h'^{Tf})\mathrm{ch}_g(\xi, h^\xi) \\ & + \mathrm{Td}_g(Tf, h'^{Tf})\widetilde{\mathrm{ch}}_g(\xi, h^\xi, h'^\xi)]. \end{aligned}$$

In particular, the class of $T_g(\omega^M, h^\xi)$ in $\widetilde{A}(B_g)$ only depends on (h^{Tf}, h^ξ).

Proof. This is [23, Theorem 2.13]. □

2.3 EQUIVARIANT BOTT-CHERN SINGULAR CURRENTS

The Bott-Chern singular current was defined by J.-M. Bismut, H. Gillet and C. Soulé in [5] in order to generalize the usual Bott-Chern secondary characteristic class to the case where one considers the resolutions of hermitian vector bundles associated to the closed immersions of complex manifolds. In [2], J.-M. Bismut generalized this topic to the equivariant case. We shall recall Bismut's construction of the equivariant Bott-Chern singular current in this subsection. Similar to the equivariant analytic torsion form, the construction itself is not very important for understanding our later arguments, we just recall it for the convenience of the reader. Bismut's construction was realized via some current valued zeta function which involves the supertraces of Quillen's superconnections. This is similar to the non-equivariant case.

As before, let g be the automorphism corresponding to an element in a compact Lie group G. Let $i: Y \to X$ be an equivariant closed immersion of G-equivariant Kähler manifolds, and let $\overline{\eta}$ be an equivariant hermitian vector bundle on Y. Assume that $\overline{\xi}.$ is a complex (of homological type) of equivariant hermitian vector bundles on X which provides a resolution of $i_*\overline{\eta}$. We denote the differential of the complex $\xi.$ by v. Note that $\xi.$ is acyclic outside Y and the homology sheaves of its restriction to Y are locally free and hence they are all vector bundles. We write $H_n = \mathcal{H}_n(\xi.\mid_Y)$ and define a $\mathbb{Z}$-graded bundle $H = \bigoplus_n H_n$. For each $y \in Y$ and $u \in TX_y$, we denote by $\partial_u v(y)$ the derivative of v at y in the direction u in any given holomorphic trivialization of $\xi.$ near y. Then the map $\partial_u v(y)$ acts on H_y as a chain map, and this action only depends on the image z of u in N_y where N stands for the normal bundle of $i(Y)$ in X. So we get a chain complex of holomorphic vector bundles $(H, \partial_z v)$.

Let π be the projection from the normal bundle N to Y, then we have a canonical identification of $\mathbb{Z}$-graded chain complexes

$$(\pi^*H, \partial_z v) \cong (\pi^*(\wedge N^\vee \otimes \eta), i_z).$$

For this, one can see [3, Section I. b]. Moreover, such an identification is an identification of G-bundles which induces a family of canonical isomorphisms $\gamma_n : H_n \cong \wedge^n N^\vee \otimes \eta$. Another way to describe these canonical isomorphisms γ_n is applying [13, Exp. VII, Lemma 2.4 and Proposition 2.5]. These two constructions coincide because they are both locally, on a suitable open covering $\{U_j\}_{j\in J}$, determined by any complex morphism over the identity map of $\eta \mid_{U_j}$ from $(\xi. \mid_{U_j}, v)$ to the minimal resolution of $\eta \mid_{U_j}$ (e.g. the Koszul resolution). The advantage of using the construction given in [13] is that it remains valid for arithmetic varieties over any base instead of the complex numbers. Later in [2], for the use of normalization, J.-M. Bismut considered the automorphism of $N^\vee$ defined by multiplying a constant $-\sqrt{-1}$, it induces an isomorphism of chain complexes

$$(\pi^*(\wedge N^\vee \otimes \eta), i_z) \cong (\pi^*(\wedge N^\vee \otimes \eta), \sqrt{-1} i_z)$$

and hence

$$(\pi^*H, \partial_z v) \cong (\pi^*(\wedge N^\vee \otimes \eta), \sqrt{-1} i_z).$$

This identification induces a family of isomorphisms $\widetilde{\gamma_n} : H_n \cong \wedge^n N^\vee \otimes \eta$. By finite dimensional Hodge theory, for each $y \in Y$, there is a canonical isomorphism

$$H_y \cong \{f \in \xi._y \mid vf = 0, v^*f = 0\}$$

where v^* is the dual of v with respect to the metrics on $\xi.$. This means that H can be regarded as a smooth $\mathbb{Z}$-graded G-equivariant subbundle of ξ so that it carries an induced G-invariant metric. On the other hand, we endow $\wedge N^\vee \otimes \eta$ with the metric induced from $\overline{N}$ and $\overline{\eta}$. J.-M. Bismut introduced the following definition.

Definition 2.13. We say that the metrics on the complex of equivariant hermitian vector bundles $\overline{\xi}.$ satisfy Bismut assumption (A) if the identification $(\pi^*H, \partial_z v) \cong (\pi^*(\wedge N^\vee \otimes \eta), \sqrt{-1} i_z)$ also identifies the metrics, it is equivalent to the condition that the identification $(\pi^*H, \partial_z v) \cong (\pi^*(\wedge N^\vee \otimes \eta), i_z)$ identifies the metrics.

Proposition 2.14. *There always exist G-invariant metrics on $\xi.$ which satisfy Bismut assumption (A) with respect to the equivariant hermitian vector bundles $\overline{N}$ and $\overline{\eta}$.*

Proof. This is [2, Proposition 3.5]. □

From now on we always suppose that the metrics on a resolution satisfy Bismut assumption (A). Let ∇^ξ be the canonical hermitian holomorphic connection on $\xi.$, then for each $u > 0$, we may define a G-invariant superconnection

$$C_u := \nabla^\xi + \sqrt{u}(v + v^*)$$

on the $\mathbb{Z}_2$-graded vector bundle ξ. Moreover, let Φ be the map $\alpha \in \wedge(T^*_{\mathbb{R}} X_g) \to (2\pi i)^{-\deg\alpha/2}\alpha \in \wedge(T^*_{\mathbb{R}} X_g)$ and denote

$$(\mathrm{Td}_g^{-1})'(\overline{N}) := \frac{\partial}{\partial b}\mid_{b=0} (\mathrm{Td}_g(b\cdot \mathrm{Id} - \frac{\Omega^{\overline{N}}}{2\pi i})^{-1})$$

where $\Omega^{\overline{N}}$ is the curvature form associated to $\overline{N}$. We recall as follows the construction of the equivariant singular current given in [2, Section VI].

Lemma 2.15. *Let N_H be the number operator on the complex ξ. i.e. it acts on ξ_j as multiplication by j, then for $s \in \mathbb{C}$ and $0 < \mathrm{Re}(s) < \frac{1}{2}$, the current valued zeta function*

$$Z_g(\overline{\xi}.)(s) := \frac{1}{\Gamma(s)}\int_0^\infty u^{s-1}[\Phi \mathrm{Tr_s}(N_H g \exp(-C_u^2)) + (\mathrm{Td}_g^{-1})'(\overline{N})\mathrm{ch}_g(\overline{\eta})\delta_{Y_g}]\mathrm{d}u$$

is well-defined on X_g and it has a meromorphic continuation to the complex plane which is holomorphic at $s = 0$.

Definition 2.16. The equivariant singular Bott-Chern current on X_g associated to the resolution $\overline{\xi}.$ is defined as

$$T_g(\overline{\xi}.) := \frac{\partial}{\partial s}\mid_{s=0} Z_g(\overline{\xi}.)(s).$$

Theorem 2.17. *The current $T_g(\overline{\xi}.)$ is a sum of (p,p)-currents and it satisfies the differential equation*

$$\mathrm{dd}^c T_g(\overline{\xi}.) = i_{g*}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}) - \sum_k (-1)^k \mathrm{ch}_g(\overline{\xi}_k).$$

Moreover, the wave front set of $T_g(\overline{\xi}.)$ is contained in $N_{g,\mathbb{R}}^\vee$ where $N_{g,\mathbb{R}}^\vee$ stands for the underlying real bundle of the dual of N_g.

Proof. This follows from [2, Theorem 6.7, Remark 6.8]. □

Finally, we recall a theorem concerning the relationship of equivariant Bott-Chern singular currents involved in a double complex. This theorem will be used to show that our definition of a general embedding morphism in equivariant arithmetic G_0-theory is reasonable.

Theorem 2.18. *Let*

$$\overline{\chi}: \quad 0 \to \overline{\eta}_n \to \cdots \to \overline{\eta}_1 \to \overline{\eta}_0 \to 0$$

be an exact sequence of equivariant hermitian vector bundles on Y. Assume that we have the following double complex consisting of resolutions of $i_*\overline{\chi}$ such that all rows are exact sequences.

$$\begin{array}{ccccccccccc} 0 & \longrightarrow & \overline{\xi}_{n,\cdot} & \longrightarrow & \cdots & \longrightarrow & \overline{\xi}_{1,\cdot} & \longrightarrow & \overline{\xi}_{0,\cdot} & \longrightarrow & 0 \\ & & \downarrow & & & & \downarrow & & \downarrow & & \\ 0 & \longrightarrow & i_*\overline{\eta}_n & \longrightarrow & \cdots & \longrightarrow & i_*\overline{\eta}_1 & \longrightarrow & i_*\overline{\eta}_0 & \longrightarrow & 0. \end{array}$$

For each k, we write $\overline{\varepsilon}_k$ for the exact sequence

$$0 \to \overline{\xi}_{n,k} \to \cdots \to \overline{\xi}_{1,k} \to \overline{\xi}_{0,k} \to 0.$$

Then we have the following equality in $\widetilde{\mathcal{U}}(X_g) := \bigoplus_{p\geq 0}(D^{p,p}(X_g)/(\mathrm{Im}\partial+\mathrm{Im}\overline{\partial}))$

$$\sum_{j=0}^{n}(-1)^j T_g(\overline{\xi}_{j,.}) = i_{g*}\frac{\widetilde{\mathrm{ch}}_g(\overline{\chi})}{\mathrm{Td}_g(\overline{N})} - \sum_k (-1)^k \widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_k).$$

Here $D^{p,p}(X_g)$ stands for the space of currents on X_g of type (p,p).

Proof. This is [21, Theorem 3.14]. □

2.4 Bismut-Ma's immersion formula

In this subsection, we shall recall Bismut-Ma's immersion formula which reflects the behaviour of the equivariant analytic torsion forms of a Kähler fibration under composition of an immersion and a submersion. By translating to the equivariant arithmetic G_0-theoretic language, such a formula can be used to measure, in arithmetic G_0-theory, the difference between a push-forward morphism and the composition formed as an embedding morphism followed by a push-forward morphism. Although Bismut-Ma's immersion formula plays a very important role in our arguments, we shall not recall its proof since it is rather long and technical.

Let $i : Y \to X$ be an equivariant closed immersion of G-equivariant Kähler manifolds. Let S be a complex manifold with the trivial G-action, and let $f : Y \to S$, $l : X \to S$ be two equivariant holomorphic submersions such that $f = l \circ i$. Assume that $\overline{\eta}$ is an equivariant hermitian vector bundle on Y and $\overline{\xi}.$ provides a resolution of $i_*\overline{\eta}$ on X whose metrics satisfy Bismut assumption (A). Let ω^Y, ω^X be the real, closed and G-invariant $(1,1)$-forms on Y, X which induce the Kähler fibrations with respect to f and l respectively. We additionally assume that ω^Y is the pull-back of ω^X so that the Kähler metric on Y is induced by the Kähler metric on X. As before, denote by N the normal bundle of $i(Y)$ in X. Consider the following exact sequence

$$\overline{\mathcal{N}}: \quad 0 \to \overline{Tf} \to \overline{Tl}\mid_Y \to \overline{N} \to 0$$

where N is endowed with the quotient metric, we shall write $\widetilde{\mathrm{Td}}_g(\overline{Tf}, \overline{Tl}\mid_Y)$ for $\widetilde{\mathrm{Td}}_g(\overline{\mathcal{N}})$ the equivariant Bott-Chern secondary characteristic class associated to $\overline{\mathcal{N}}$. It satisfies the following differential equation

$$\mathrm{dd}^c\widetilde{\mathrm{Td}}_g(\overline{Tf}, \overline{Tl}\mid_Y) = \mathrm{Td}_g(Tf, h^{Tf})\mathrm{Td}_g(\overline{N}) - \mathrm{Td}_g(Tl\mid_Y, h^{Tl}).$$

For simplicity, we shall suppose that in the resolution $\xi.$, ξ_j are all $l-$acyclic and moreover η is $f-$acyclic. By an easy argument of long exact sequence, we have the following exact sequence

$$\Xi: \quad 0 \to l_*(\xi_m) \to l_*(\xi_{m-1}) \to \ldots \to l_*(\xi_0) \to f_*\eta \to 0.$$

By the semi-continuity theorem, all the elements in the exact sequence above are vector bundles. In this case, we recall the definition of the L^2-metrics on direct images precisely as follows. We just take f_*h^η as an example. Note that the semi-continuity theorem implies that the natural map

$$(R^0f_*\eta)_s \to H^0(Y_s, \eta\mid_{Y_s})$$

is an isomorphism for every point $s \in S$ where Y_s stands for the fibre over s. We may endow $H^0(Y_s, \eta\mid_{Y_s})$ with a L^2-metric given by the formula

$$< u, v >_{L^2} := \frac{1}{(2\pi)^{d_s}} \int_{Y_s} h^\eta(u, v) \frac{{\omega^Y}^{d_s}}{d_s!}$$

where d_s is the complex dimension of the fibre Y_s. It can be shown that these metrics depend on s in a C^∞ manner (cf. [9, p.278]) and hence define a hermitian metric on $f_*\eta$. We shall denote it by f_*h^η.

In order to understand the statement of Bismut-Ma's immersion formula, we still have to recall an important concept defined by J.-M. Bismut, the equivariant R-genus. Let W be a G-equivariant complex manifold, and let $\overline{E}$ be an equivariant hermitian vector bundle on W. For $\zeta \in S^1$ and $s > 1$ consider the zeta function

$$L(\zeta, s) = \sum_{k=1}^{\infty} \frac{\zeta^k}{k^s}$$

and its meromorphic continuation to the whole complex plane. Define the formal power series in x

$$\widetilde{R}(\zeta, x) := \sum_{n=0}^{\infty} \big(\frac{\partial L}{\partial s}(\zeta, -n) + L(\zeta, -n) \sum_{j=1}^{n} \frac{1}{2j}\big) \frac{x^n}{n!}.$$

DEFINITION 2.19. The Bismut equivariant R-genus of an equivariant hermitian vector bundle $\overline{E}$ with $\overline{E}\mid_{X_g} = \sum_\zeta \overline{E}_\zeta$ is defined as

$$R_g(\overline{E}) := \sum_{\zeta \in S^1} \big(\mathrm{Tr}\widetilde{R}(\zeta, -\frac{\Omega^{\overline{E}_\zeta}}{2\pi i}) - \mathrm{Tr}\widetilde{R}(1/\zeta, \frac{\Omega^{\overline{E}_\zeta}}{2\pi i})\big)$$

where $\Omega^{\overline{E}_\zeta}$ is the curvature form associated to $\overline{E}_\zeta$. Actually, the class of $R_g(\overline{E})$ in $\widetilde{A}(X_g)$ is independent of the metric and we just write $R_g(E)$ for it. Furthermore, the class $R_g(\cdot)$ is additive.

THEOREM 2.20. *(Immersion formula) Let notations and assumptions be as* *above. Then the equality*

$$\sum_{i=0}^{m}(-1)^i T_g(\omega^X,h^{\xi_i})-T_g(\omega^Y,h^\eta)+\widetilde{\mathrm{ch}}_g(\Xi,h^{L^2})$$
$$=\int_{X_g/S}\mathrm{Td}_g(Tl,h^{Tl})T_g(\overline{\xi}.)+\int_{Y_g/S}\frac{\widetilde{\mathrm{Td}}_g(\overline{Tf},\overline{Tl}\mid_Y)}{\mathrm{Td}_g(\overline{N})}\mathrm{ch}_g(\overline{\eta})$$
$$+\int_{X_g/S}\mathrm{Td}_g(Tl)R_g(Tl)\sum_{i=0}^{m}(-1)^i\mathrm{ch}_g(\xi_i)-\int_{Y_g/S}\mathrm{Td}_g(Tf)R_g(Tf)\mathrm{ch}_g(\eta)$$

holds in $\widetilde{A}(S)$.

Proof. This is the combination of [8, Theorem 0.1 and 0.2], the main theorems in that paper. □

3 A vanishing theorem for equivariant closed immersions

3.1 The statement

By a projective manifold we shall understand a compact complex manifold which is projective algebraic, that means a projective manifold is the complex analytic space $X(\mathbb{C})$ associated to a smooth projective variety X over $\mathbb{C}$ (cf. [17, Appendix B]). Let μ_n be the diagonalisable group variety over $\mathbb{C}$ associated to $\mathbb{Z}/n\mathbb{Z}$. We say X is μ_n-equivariant if it admits a μ_n-projective action, this means the associated projective manifold $X(\mathbb{C})$ admits an action by the group of complex n-th roots of unity. Denote by X_{μ_n} the fixed point subscheme of X, by GAGA principle, $X_{\mu_n}(\mathbb{C})$ is equal to $X(\mathbb{C})_g$ where g is the automorphism on $X(\mathbb{C})$ corresponding to a fixed primitive n-th root of unity. If no confusion arises, we shall not distinguish between X and $X(\mathbb{C})$ as well as X_{μ_n} and X_g. Since the classical arguments of locally free resolutions may not be compatible with the equivariant setting, we summarize some crucial facts we need as follows.
(i). Every equivariant coherent sheaf on an equivariantly projective scheme is an equivariant quotient of an equivariant locally free coherent sheaf.
(ii). Every equivariant coherent sheaf on an equivariantly projective scheme admits an equivariant locally free resolution. It is finite if the equivariant scheme is regular.
(iii). An exact sequence of equivariant coherent sheaves on an equivariantly projective scheme admits an exact sequence of equivariant locally free resolutions.
(iv). Any two equivariant locally free resolutions of an equivariant coherent sheaf on an equivariantly projective scheme can be dominated by a third one.
Now let $i: Y\to X$ be a μ_n-equivariant closed immersion of projective manifolds with normal bundle N. Let S be a projective manifold with the trivial μ_n-action and let $h: X\to S$ be an equivariant holomorphic submersion whose

restriction $f : Y \to S$ is an equivariant holomorphic submersion. According to our assumptions, we may define a Kähler fibration with respect to h by choosing a $\mu_n(\mathbb{C})$-invariant Kähler form ω^X on X. By restricting ω^X to Y we obtain a Kähler fibration with respect to f. The same thing goes to $h_g : X_g \to S$ and $f_g : Y_g \to S$. Let $\overline{\eta}$ be an equivariant hermitian holomorphic vector bundle on Y, assume that $(\overline{\xi.}, v)$ is a complex of equivariant hermitian vector bundles on X which provides a resolution of $i_*\overline{\eta}$, whose metrics satisfy Bismut assumption (A).

Write N_g for the 0-degree part of $N\mid_{Y_g}$ which is isomorphic to the normal bundle of $i_g(Y_g)$ in X_g and denote by F the orthogonal complement of N_g. According to [13, Exp. VII, Lemma 2.4 and Proposition 2.5] we know that there exists a canonical isomorphism from the homology sheaf $H(\xi.\mid_{X_g})$ to $i_{g*}(\wedge^\cdot F^\vee \otimes \eta\mid_{Y_g})$ which is equivariant. Then the restriction of $(\xi., v)$ to X_g can always split into a series of short exact sequences in the following way:

$$(*) : \quad 0 \to \mathrm{Im} \to \mathrm{Ker} \to i_{g*}(\wedge^\cdot F^\vee \otimes \eta\mid_{Y_g}) \to 0$$

and

$$(**) : \quad 0 \to \mathrm{Ker} \to \xi.\mid_{X_g} \to \mathrm{Im} \to 0.$$

Suppose that $\wedge^\cdot F^\vee \otimes \eta\mid_{Y_g}$ and $\xi.\mid_{X_g}$ are all acyclic (higher direct images vanish). Then according to an easy argument of long exact sequence, these short exact sequences $(*)$ and $(**)$ induce a series of short exact sequences of direct images:

$$\mathcal{H}(*) : \quad 0 \to R^0h_{g*}(\mathrm{Im}) \to R^0h_{g*}(\mathrm{Ker}) \to R^0f_{g*}(\wedge^\cdot F^\vee \otimes \eta\mid_{Y_g}) \to 0$$

and

$$\mathcal{H}(**) : \quad 0 \to R^0h_{g*}(\mathrm{Ker}) \to R^0h_{g*}(\xi.\mid_{X_g}) \to R^0h_{g*}(\mathrm{Im}) \to 0.$$

By semi-continuity theorem, all elements in the exact sequences above are vector bundles. We endow $R^0h_{g*}(\xi.\mid_{X_g})$ and $R^0f_{g*}(\wedge^\cdot F^\vee \otimes \eta\mid_{Y_g})$ with the L^2-metrics which are induced by the metrics on $\xi.$, η and F. Here the normal bundle N admits the quotient metric induced from the exact sequence

$$0 \to Tf \to Th\mid_Y \to N \to 0$$

and the bundle F admits the metric induced by the metric on N. Moreover, we endow $R^0h_{g*}(\mathrm{Im})$ and $R^0h_{g*}(\mathrm{Ker})$ with the metrics induced by the L^2-metrics of $R^0h_{g*}(\xi.\mid_{X_g})$ so that $\mathcal{H}(*)$ and $\mathcal{H}(**)$ become short exact sequences of equivariant hermitian vector bundles. Denote by $\widetilde{\mathrm{ch}}_g(\overline{\xi.}, \overline{\eta})$ the alternating sum of the equivariant secondary Bott-Chern characteristic classes of $\mathcal{H}(*)$ and $\mathcal{H}(**)$ such that it satisfies the following differential equation

$$\mathrm{dd}^c\widetilde{\mathrm{ch}}_g(\overline{\xi.}, \overline{\eta}) = \sum_j (-1)^j \mathrm{ch}_g(R^0f_{g*}(\wedge^j \overline{F}^\vee \otimes \overline{\eta}\mid_{Y_g})) - \sum_j (-1)^j \mathrm{ch}_g(R^0h_{g*}(\overline{\xi}_j\mid_{X_g})).$$

Now the difference

$$\begin{aligned}\delta(i,\overline{\eta},\overline{\xi}.) :=& \widetilde{\mathrm{ch}}_g(\overline{\xi}.,\overline{\eta}) - \sum_k (-1)^k T_g(\omega^{Y_g}, h^{\wedge^k F^\vee\otimes\eta|_{Y_g}}) \\ &+ \sum_k (-1)^k T_g(\omega^{X_g}, h^{\xi_k|_{X_g}}) - \int_{X_g/S} T_g(\overline{\xi}.)\mathrm{Td}(\overline{Th_g}) \\ &- \int_{Y_g/S} \mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g) \\ &- \int_{Y_g/S} \mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Th_g}\mid_{Y_g})\end{aligned}$$

makes sense and it is an element in $\bigoplus_{p\geq 0} A^{p,p}(S)/(\mathrm{Im}\partial + \mathrm{Im}\overline{\partial})$. Here the symbols $T_g(\cdot)$ in the summations stand for analytic torsion forms introduced in Section 2.1, the symbol $T_g(\overline{\xi}.)$ in the integral is the equivariant Bott-Chern singular current introduced in Section 2.2.

The vanishing theorem for equivariant closed immersions can be formulated as the following.

Theorem 3.1. *Let $i : Y \to X$ be an equivariant closed immersion of projective manifolds, and let S be a projective manifold with the trivial μ_n-action. Assume that we are given two equivariant holomorphic submersions $f : Y \to S$ and $h : X \to S$ such that $f = h \circ i$. Then X admits an equivariant hermitian very ample invertible sheaf $\overline{\mathcal{L}}$ relative to the morphism h, and for any equivariant hermitian resolution $0 \to \overline{\xi}_m \to \cdots \overline{\xi}_1 \to \overline{\xi}_0 \to i_*\overline{\eta} \to 0$ we have*

$$\delta(i, \overline{\eta}\otimes i^*\overline{\mathcal{L}}^{\otimes n}, \overline{\xi}.\otimes\overline{\mathcal{L}}^{\otimes n}) = 0 \qquad \textit{for} \quad n \gg 0.$$

Here the metrics on the resolution are supposed to satisfy Bismut assumption (A).

3.2 Deformation to the normal cone

To prove the vanishing theorem for closed immersions, we use a geometric construction called the deformation to the normal cone which allows us to deform a resolution of hermitian vector bundle associated to a closed immersion of projective manifolds to a simpler one. The δ-difference of this new simpler resolution is much easier to compute.

Let $i : Y \hookrightarrow X$ be a closed immersion of projective manifolds with normal bundle $N_{X/Y}$. For a vector bundle E on X or Y, the notation $\mathbb{P}(E)$ will stand for the projective space bundle $\mathrm{Proj}(\mathrm{Sym}(E^\vee))$.

Definition 3.2. The deformation to the normal cone $W(i)$ of the immersion i is the blowing up of $X \times \mathbb{P}^1$ along $Y \times \{\infty\}$. We shall just write W for $W(i)$ if there is no confusion about the immersion.

There are too many geometric objects and morphisms appearing in the construction of the deformation to the normal cone, we have to fix various notations in a clear way. We denote by p_X (resp. p_Y) the projection $X\times\mathbb{P}^1\to X$ (resp. $Y\times\mathbb{P}^1\to Y$) and by π the blow-down map $W\to X\times\mathbb{P}^1$. We also denote by q_X (resp. q_Y) the projection $X\times\mathbb{P}^1\to\mathbb{P}^1$ (resp. $Y\times\mathbb{P}^1\to\mathbb{P}^1$) and by q_W the composition $q_X\circ\pi$. It is well known that the map q_W is flat and for $t\in\mathbb{P}^1$, we have

$$q_W^{-1}(t)\cong\begin{cases} X\times\{t\}, & \text{if } t\neq\infty,\\ P\cup\widetilde{X}, & \text{if } t=\infty,\end{cases}$$

where $\widetilde{X}$ is isomorphic to the blowing up of X along Y and P is isomorphic to the projective completion of $N_{X/Y}$ i.e. the projective space bundle $\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)$. Denote the canonical projection from $\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)$ to Y by π_P, then the morphism $\mathcal{O}_Y\to N_{X/Y}\oplus\mathcal{O}_Y$ induces a canonical section $i_\infty: Y\hookrightarrow\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)$ which is called the zero section embedding. Moreover, let $j: Y\times\mathbb{P}^1\to W$ be the canonical closed immersion induced by $i\times\mathrm{Id}$, then the component $\widetilde{X}$ doesn't meet $j(Y\times\mathbb{P}^1)$ and the intersection of $j(Y\times\mathbb{P}^1)$ with P is exactly the image of Y under the section i_∞.

The advantage of the construction of the deformation to the normal cone is that we may control the rational equivalence class of the fibres $q_W^{-1}(t)$. More precisely, in the language of line bundles, we have the isomorphisms $\mathcal{O}(X)\cong\mathcal{O}(P+\widetilde{X})\cong\mathcal{O}(P)\otimes\mathcal{O}(\widetilde{X})$ which is an immediate consequence of the isomorphism $\mathcal{O}(0)\cong\mathcal{O}(\infty)$ on $\mathbb{P}^1$.

On $P=\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)$, there exists a tautological exact sequence

$$0\to\mathcal{O}(-1)\to\pi_P^*(N_{X/Y}\oplus\mathcal{O}_Y)\to Q\to 0$$

where Q is the tautological quotient bundle. This exact sequence and the inclusion $\mathcal{O}_P\to\pi_P^*(N_{X/Y}\oplus\mathcal{O}_Y)$ induce a section $\sigma:\mathcal{O}_P\to Q$ which vanishes along the zero section $i_\infty(Y)$. By duality we get a morphism $Q^\vee\to\mathcal{O}_P$, and this morphism induces the following exact sequence

$$0\to\wedge^nQ^\vee\to\cdots\to\wedge^2Q^\vee\to Q^\vee\to\mathcal{O}_P\to i_{\infty*}\mathcal{O}_Y\to 0$$

where n is the rank of Q. Note that i_∞ is a section of π_P i.e. $\pi_P\circ i_\infty=\mathrm{Id}$, the projection formula implies the following definition.

Definition 3.3. For any vector bundle η on Y, the following complex of vector bundles

$$0\to\wedge^nQ^\vee\otimes\pi_P^*\eta\to\cdots\to\wedge^2Q^\vee\otimes\pi_P^*\eta\to Q^\vee\otimes\pi_P^*\eta\to\pi_P^*\eta\to 0$$

provides a resolution of $i_{\infty*}\eta$ on P. This complex is called the Koszul resolution of $i_{\infty*}\eta$ and will be denoted by $\kappa(\eta,N_{X/Y})$. If the normal bundle $N_{X/Y}$ admits some hermitian metric, then the tautological exact sequence induces a hermitian metric on Q. If, moreover, the bundle η also admits a hermitian metric, then the Koszul resolution is a complex of hermitian vector bundles and will be denoted by $\overline{\kappa}(\overline{\eta},\overline{N}_{X/Y})$.

Now, assume that X is a μ_n-equivariant projective manifold and E is an equivariant locally free sheaf on X. Then according to [20, (1.4) and (1.5)], $\mathbb{P}(E)$ admits a canonical μ_n-equivariant structure such that the projection map $\mathbb{P}(E) \to X$ is equivariant and the canonical bundle $\mathcal{O}(1)$ admits an equivariant structure. Moreover, let $Y \to X$ be an equivariant closed immersion of projective manifolds, according to [20, (1.6)] the action of μ_n on X can be extended to the blowing up $\mathrm{Bl}_Y X$ such that the blow-down map is equivariant and the canonical bundle $\mathcal{O}(1)$ admits an equivariant structure. So by endowing $\mathbb{P}^1$ with the trivial μ_n-action, the construction of the deformation to the normal cone described above is compatible with the equivariant setting.
For the use of our later arguments, the Kähler metric chosen on W should be well controlled on the fibres of the deformation. For this purpose, it is necessary to introduce the following definition.

Definition 3.4. (Rössler) A metric h on W is said to be normal to the deformation if
(a). it is invariant and Kähler;
(b). the restriction $h\mid_{j_{g*}(Y_g\times\mathbb{P}^1)}$ is a product $h'\times h''$, where h' is a Kähler metric on Y_g and h'' is a Kähler metric on $\mathbb{P}^1$;
(c). the intersections of $X\times\{0\}$ with $j_*(Y\times\mathbb{P}^1)$ and of P with $j_*(Y\times\mathbb{P}^1)$ are orthogonal at the fixed points.

Lemma 3.5. *For any μ_n-invariant Kähler metric h^X on X which induces an invariant Kähler metric h^Y on Y, there exists a metric h^W on W which is normal to the deformation and the restriction of h^W to $X\cong X\times\{0\}$ (resp. $Y\cong Y\times\{\infty\}$) is exactly h^X (resp. h^Y). Moreover, we may require that the hermitian normal bundles $\overline{N}_{Y\times\mathbb{P}^1/Y\times\{0\}}$ and $\overline{N}_{Y\times\mathbb{P}^1/Y\times\{\infty\}}$ are both isometric to the trivial bundles with trivial metrics.*

Proof. The existence of the metric which is normal to the deformation is the content of [21, Lemma 6.13] and [28, Lemma 6.14], such a metric is constructed via the Grassmannian graph construction. Roughly speaking, according to another description of the deformation to the normal cone via the Grassmannian graph construction, we have an embedding $W\to X\times\mathbb{P}^r\times\mathbb{P}^1$ and the metric h^W is the μ_n-average of the restriction of a product metric on $X\times\mathbb{P}^r\times\mathbb{P}^1$ (cf. [28, Lemma 6.14]). When we endow X in the product with the metric h^X, the requirements on restrictions are automatically satisfied since h^X is μ_n-invariant. To fulfill the requirements on hermitian normal bundles, we may just choose the Fubini-Study metric on $\mathbb{P}^1$. □

We summarize some very important results about the application of the deformation to the normal cone as follows. Their proofs can be found in [21, Section 2 and 6.2].

Theorem 3.6. *Let $i: Y\to X$ be an equivariant closed immersion of equivariant projective manifolds, and let $W=W(i)$ be the deformation to the normal cone of i. Assume that $\overline{\eta}$ is an equivariant hermitian vector bundle on Y. Then*

(i). there exists an equivariant hermitian resolution of $j_*p_Y^*(\overline{\eta})$ on W, whose metrics satisfy Bismut assumption (A) and whose restriction to $\widetilde{X}$ is equivariantly and orthogonally split;
(ii). the natural morphism from the deformation to the normal cone $W(i_g)$ to the fixed point submanifold $W(i)_g$ is a closed immersion, this closed immersion induces the closed immersions $\mathbb{P}(N_{X_g/Y_g}\oplus\mathcal{O}_{Y_g})\to\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)_g$ and $\widetilde{X_g}\to\widetilde{X}_g$;
(iii). the fixed point submanifold of $\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)$ is $\mathbb{P}(N_{X_g/Y_g}\oplus\mathcal{O}_{Y_g})\coprod_{\zeta\neq1}\mathbb{P}((N_{X/Y})_\zeta)$;
(iv). the closed immersion $i_{\infty,g}$ factors through $\mathbb{P}(N_{X_g/Y_g}\oplus\mathcal{O}_{Y_g})$ and the other components $\mathbb{P}((N_{X/Y})_\zeta)$ don't meet Y. Hence the complex $\kappa(\mathcal{O}_Y,N_{X/Y})_g$, obtained by taking the 0-degree part of the Koszul resolution, provides a resolution of $\mathcal{O}_{Y_g}$ on $\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)_g$.

3.3 Proof of the vanishing theorem

We shall first prove the first part of the vanishing theorem for closed immersions i.e. the existence of an equivariant hermitian very ample invertible sheaf on X which is relative to the morphism $h:X\to S$. Generally speaking, such an invertible sheaf can be constructed rather easily since X admits a μ_n-projective action and the μ_n-action on S is supposed to be trivial, but for the whole proof of the vanishing theorem we would like to construct a special one which is the pull-back of some equivariant hermitian very ample invertible sheaf on $W(i)$ under the identification $X\cong X\times\{0\}$. Our starting point is the following.

Definition 3.7. Let M be a μ_n-projective manifold, and let $\mathbb{P}^n_M$ be some relative projective space over M. A μ_n-action on $\mathbb{P}^n_M$ arising from some μ_n-action on the free sheaf $\mathcal{O}_M^{\oplus n+1}$ via the functorial properties of the Proj symbol will be called a global μ_n-action.

The advantage of considering global μ_n-action is that on a projective space which admits a global μ_n-action the twisted line bundle $\mathcal{O}(1)$ is naturally μ_n-equivariant.

Lemma 3.8. *The morphism $h:X\to S$ factors though some relative projective space $\mathbb{P}^r_S$ which admits a global μ_n-action.*

Proof. By assumption, X admits a μ_n-projective action. Then [21, Lemma 2.4 and 2.5] imply that there exists an equivariant closed immersion from X to some projective space $\mathbb{P}^r$ endowed with a global action. By using the universal property of fibre product, we obtain a morphism from X to $\mathbb{P}^r_S=S\times\mathbb{P}^r$ which is equivariant. Moreover, this morphism is clearly a closed immersion. Since the action on S is trivial, the induced action on the fibre product $S\times\mathbb{P}^r$ is still global. So we are done. □

Lemma 3.9. *Let $l:W(i)\to S$ be the composition $h\circ p_X\circ\pi$. Then $W(i)$ admits an equivariant very ample invertible sheaf $\mathcal{L}$ which is relative to l.*

Proof. By Lemma 3.8, $h : X \to S$ factors through some relative projective space $\mathbb{P}^r_S$ which admits a global μ_n-action. So X admits an equivariant very ample invertible sheaf relative to h. Since the μ_n-action on S is supposed to be trivial, $\mathbb{P}^1_X = X \times \mathbb{P}^1 \cong X \times_S \mathbb{P}^1_S$ also admits an equivariant very ample invertible sheaf relative to the morphism $h \circ p_X$ which is denoted by $\mathcal{G}$. Moreover, by construction, $W(i)$ admits a very ample invertible sheaf $\mathcal{O}_W(1) \otimes \pi^*\mathcal{G}^{\otimes b}$ for some $b \geq 0$ which is relative to the blow-down map π (cf. [17, II. Proposition 7.10]). Assume that $\mathbb{P}^1_X \times_S \mathbb{P}^m_S$ is the relative projective space associated to $\mathcal{O}_W(1) \otimes \pi^*\mathcal{G}^{\otimes b}$, and that $\mathbb{P}^n_S$ is the relative projective space associated to $\mathcal{G}$. Then the very ample invertible sheave on $\mathbb{P}^1_X \times_S \mathbb{P}^m_S$ with respect to the embedding

$$\mathbb{P}^1_X \times_S \mathbb{P}^m_S \hookrightarrow \mathbb{P}^n_S \times_S \mathbb{P}^m_S$$

can be written as $\mathcal{G} \boxtimes \mathcal{O}_{\mathbb{P}^m_S}(1)$ whose restriction to $W(i)$ is equal to $\mathcal{O}_W(1) \otimes \pi^*\mathcal{G}^{\otimes b+1}$. Therefore, $\mathcal{O}_W(1) \otimes \pi^*\mathcal{G}^{\otimes b+1}$ is a very ample invertible sheaf on $W(i)$ relative to $l : W(i) \to S$, this invertible sheaf is clearly equivariant. □

From now on, we shall fix the equivariant very ample invertible sheaf $\mathcal{L}$ constructed in Lemma 3.9. We also fix a μ_n-invariant hermitian metric on $\mathcal{L}$, note that this metric always exists according to an argument of partition of unity. When we deal with the tensor product of a coherent sheaf $\mathcal{F}$ with some power $\mathcal{L}^{\otimes n}$, we just write it as $\mathcal{F}(n)$ for simplicity. Before we give the proof of the rest of the vanishing theorem, we shall recall the concept of equivariant standard complex and some technical results.

Definition 3.10. Let S be a projective manifold and let $\overline{\xi}.$ be a bounded complex of hermitian vector bundles on S. We say $\overline{\xi}.$ is a standard complex if the homology sheaves of $\overline{\xi}.$ are all locally free and they are endowed with some hermitian metrics. We shall write a standard complex as $(\overline{\xi}., h^H)$ to emphasize the choice of the metrics on the homology sheaves.

Definition 3.11. Let S be an equivariant projective manifold. An equivariant standard complex on S is a bounded complex of equivariant hermitian vector bundles on S whose restriction to S_g is standard and the metrics on the homology sheaves are g-invariant. Again we shall write an equivariant standard complex as $(\overline{\xi}., h^H)$ to emphasize the choice of the metrics on the homology sheaves.

Due to [29, Theorem 5.9], to every equivariant standard complex $(\overline{\xi}., h^H)$ on an equivariant projective manifold S, there is a unique axiomatical way to associate an element $\widetilde{\mathrm{ch}}_g(\overline{\xi}., h^H)$ in $\bigoplus_{p \geq 0} A^{p,p}(S_g)/(\mathrm{Im}\partial + \mathrm{Im}\overline{\partial})$ which satisfies the differential equation

$$\mathrm{dd}^c \widetilde{\mathrm{ch}}_g(\overline{\xi}., h^H) = \sum_j (-1)^j \mathrm{ch}_g(H_j(\overline{\xi}. \mid_{S_g})) - \sum_j (-1)^j \mathrm{ch}_g(\overline{\xi}_j).$$

Let $0 \to \overline{\xi.}' \to \overline{\xi.} \to \overline{\xi.}'' \to 0$ be a short exact sequence of equivariant standard complexes on S. Then by restricting to the fixed point submanifold S_g, we get a short exact sequence of standard complexes $0 \to \overline{\xi.}' \mid_{S_g} \to \overline{\xi.} \mid_{S_g} \to \overline{\xi.}'' \mid_{S_g} \to 0$. Hence we obtain a long exact sequence of homology sheaves of these three standard complexes. We shall make a stronger assumption. Suppose that for any $j \geq 0$, we have short exact sequence $0 \to H_j(\overline{\xi.}' \mid_{S_g}) \to H_j(\overline{\xi.} \mid_{S_g}) \to H_j(\overline{\xi.}'' \mid_{S_g}) \to 0$ which is denoted by $\overline{\chi}_j$. Moreover, for any $j \geq 0$, denote by $\overline{\varepsilon}_j$ the short exact sequence $0 \to \overline{\xi}_j' \to \overline{\xi}_j \to \overline{\xi}_j'' \to 0$.

LEMMA 3.12. *Let notations and assumptions be as above. The identity*

$$\widetilde{\mathrm{ch}}_g(\overline{\xi.}', h^H) - \widetilde{\mathrm{ch}}_g(\overline{\xi.}, h^H) + \widetilde{\mathrm{ch}}_g(\overline{\xi.}'', h^H) = \sum (-1)^j \widetilde{\mathrm{ch}}_g(\overline{\chi}_j) - \sum (-1)^j \widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j)$$

holds in $\bigoplus_{p \geq 0} A^{p,p}(S_g)/(\mathrm{Im}\partial + \mathrm{Im}\overline{\partial})$.

Proof. On S_g, every equivariant standard complex $(\overline{\xi.}, h^H)$ splits into a series of short exact sequences of equivariant hermitian vector bundles in the following way

$$0 \to \overline{\mathrm{Im}} \to \overline{\mathrm{Ker}} \to \overline{H.} \to 0$$

and

$$0 \to \overline{\mathrm{Ker}} \to \overline{\xi.} \mid_{S_g} \to \overline{\mathrm{Im}} \to 0.$$

According to the argument given after [29, Remark 5.10], $\widetilde{\mathrm{ch}}_g(\overline{\xi.}, h^H)$ is equal to the alternating sum of the equivariant Bott-Chern secondary characteristic classes of the short exact sequences above. Now since we have supposed that $0 \to H_j(\overline{\xi.}' \mid_{S_g}) \to H_j(\overline{\xi.} \mid_{S_g}) \to H_j(\overline{\xi.}'' \mid_{S_g}) \to 0$ are all exact, by using Snake lemma, we know that $0 \to \mathrm{Im}(\overline{\xi.}' \mid_{S_g}) \to \mathrm{Im}(\overline{\xi.} \mid_{S_g}) \to \mathrm{Im}(\overline{\xi.}'' \mid_{S_g}) \to 0$ and $0 \to \mathrm{Ker}(\overline{\xi.}' \mid_{S_g}) \to \mathrm{Ker}(\overline{\xi.} \mid_{S_g}) \to \mathrm{Ker}(\overline{\xi.}'' \mid_{S_g}) \to 0$ are also all exact sequences. Then the identity in the statement of this lemma immediately follows from the construction of $\widetilde{\mathrm{ch}}_g(\overline{\xi.}, h^H)$ and the additivity property of the equivariant Bott-Chern secondary characteristic classes. ☐

COROLLARY 3.13. *Let* $0 \to \overline{\xi.}^{(m)} \to \cdots \to \overline{\xi.}^{(1)} \to \overline{\xi.}^{(0)} \to 0$ *be an exact sequence of equivariant standard complexes on* S *such that for every* $j \geq 0$, $0 \to H_j(\overline{\xi.}^{(m)} \mid_{S_g}) \to \cdots \to H_j(\overline{\xi.}^{(1)} \mid_{S_g}) \to H_j(\overline{\xi.}^{(0)} \mid_{S_g}) \to 0$ *is exact. Then the identity*

$$\sum_{k=0}^{m} (-1)^k \widetilde{\mathrm{ch}}_g(\overline{\xi.}^{(k)}, h^H) = \sum (-1)^j \widetilde{\mathrm{ch}}_g(\overline{\chi}_j) - \sum (-1)^j \widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j)$$

holds in $\bigoplus_{p \geq 0} A^{p,p}(S_g)/(\mathrm{Im}\partial + \mathrm{Im}\overline{\partial})$.

Proof. We claim that for every $1 \leq k \leq m$, the kernel of the complex morphism $\overline{\xi.}^{(k)} \to \overline{\xi.}^{(k-1)}$ is still an equivariant standard complex on S. It is clear that we only need to prove this for $k = 1$. Firstly, the kernel of $\overline{\xi.}^{(1)} \to \overline{\xi.}^{(0)}$ is a complex of equivariant hermitian vector bundles, let's denote it by $\overline{K}$. By restricting to

S_g and using an argument of long exact sequence, we know that the homology sheaves of $\overline{K}\mid_{S_g}$ are all equivariant hermitian vector bundles since for any $j\geq 0$ the bundle morphism $H_j(\overline{\xi.}^{(1)}\mid_{S_g})\to H_j(\overline{\xi.}^{(0)}\mid_{S_g})$ is already surjective. Therefore, the assumption of exactness on homologies implies that we can split $0\to\overline{\xi.}^{(m)}\to\cdots\to\overline{\xi.}^{(1)}\to\overline{\xi.}^{(0)}\to 0$ into a series of short exact sequences of equivariant standard complexes, so the identity in the statement of this corollary follows from Lemma 3.12. □

Remark 3.14. A generalized version of Corollary 3.13, in which the exact sequence of (equivariant) standard complexes is replaced by an (equivariant) double standard complex was obtained in Xiaonan Ma's Ph.D thesis (cf. [24]) where more discussions concerning spectral sequences were involved. Anyway, for arithmetical reason, we only need these special versions as in Lemma 3.12 and Corollary 3.13.

Now we turn back to our proof of the vanishing theorem. As before, let $W=W(i)$ be the deformation to the normal cone associated to an equivariant closed immersion of projective manifolds $i:Y\to X$. For simplicity, denote by P_g^0 the projective space bundle $\mathbb{P}(N_{X_g/Y_g}\oplus\mathcal{O}_{Y_g})$. Moreover, given an invariant Kähler metric on X, we fix an invariant Kähler metric on W which is constructed in Lemma 3.5. In this situation, all normal bundles appearing in the construction of the deformation to the normal cone will be endowed with the quotient metrics. We recall the following lemma.

Lemma 3.15. *Over $W(i_g)$, there are hermitian metrics on $\mathcal{O}(X_g)$, $\mathcal{O}(P_g^0)$ and $\mathcal{O}(\widetilde{X_g})$ such that the isometry $\overline{\mathcal{O}}(X_g)\cong\overline{\mathcal{O}}(P_g^0)\otimes\overline{\mathcal{O}}(\widetilde{X_g})$ holds and such that the restriction of $\overline{\mathcal{O}}(X_g)$ to X_g yields the metric of $N_{W(i_g)/X_g}$, the restriction of $\overline{\mathcal{O}}(\widetilde{X_g})$ to $\widetilde{X_g}$ yields the metric of $N_{W(i_g)/\widetilde{X_g}}$ and the restriction of $\overline{\mathcal{O}}(P_g^0)$ to P_g^0 induces the metric of $N_{W(i_g)/P_g^0}$.*

Proof. This is [21, Lemma 6.15]. □

Definition 3.16. Let $\overline{\eta}$ be an equivariant hermitian vector bundle on Y, we say that a resolution

$$\overline{\Xi}:\quad 0\to\overline{\widetilde{\xi}}_m\to\cdots\to\overline{\widetilde{\xi}}_0\to j_*p_Y^*(\overline{\eta})\to 0$$

satisfies the condition (T) if
(i). the metrics on $\widetilde{\xi}.$ satisfy Bismut assumption (A);
(ii). the restriction of $\overline{\Xi}$ to $\widetilde{X}$ is an equivariantly and orthogonally split exact sequence;
(iii). the restrictions of $\overline{\Xi}_\triangledown$ to $W(i_g)$, X_g, P_g^0, $\widetilde{X_g}$ and $P_g^0\cap\widetilde{X_g}$ are complexes with l-acyclic elements and l-acyclic homologies, here $\overline{\Xi}_\triangledown$ is the complex of hermitian vector bundles obtained by omitting the last term $j_*p_Y^*(\overline{\eta})$ in $\overline{\Xi}$;

(iv). the tensor products $\overline{\Xi}_\nabla\mid_{W(i_g)}\otimes\overline{\mathcal{O}}(-X_g)$, $\overline{\Xi}_\nabla\mid_{W(i_g)}\otimes\overline{\mathcal{O}}(-P_g^0)$ and $\overline{\Xi}_\nabla\mid_{W(i_g)}\otimes\overline{\mathcal{O}}(-\widetilde{X_g})$ are complexes with l-acyclic elements and l-acyclic homologies.

From Theorem 3.6 (i), we already know that there always exists a resolution of $j_*p_Y^*(\overline{\eta})$ which satisfies the conditions (i) and (ii) in Definition 3.16. Let $\overline{\Xi}$ be such a resolution, we have the following.

Proposition 3.17. *For $n\gg 0$, $\overline{\Xi}(n)$ satisfies the condition (T).*

Proof. The reason is that $W(i_g)$, X_g, P_g^0, $\widetilde{X_g}$ and $P_g^0\cap\widetilde{X_g}$ are all closed submanifolds of W. □

It is well known that both two squares in the following deformation diagram

$$\begin{array}{ccccc}
Y\times\{0\} & \xrightarrow{s_0} & Y\times\mathbb{P}^1 & \xleftarrow{s_\infty} & Y\times\{\infty\} \\
\downarrow{\scriptstyle i} & & \downarrow{\scriptstyle j} & & \downarrow{\scriptstyle i_\infty} \\
X\times\{0\} & \longrightarrow & W & \longleftarrow & \mathbb{P}(N_{X/Y}\oplus N_{\mathbb{P}^1/\infty})
\end{array}$$

are Tor-independent. Moreover, according to our choices of the Kähler metrics, we may identify $Y\times\{0\}$ with Y, $X\times\{0\}$ with X, $Y\times\{\infty\}$ with Y and $\mathbb{P}(N_{X/Y}\oplus N_{\mathbb{P}^1/\infty})$ with $P=\mathbb{P}(N_{X/Y}\oplus\mathcal{O}_Y)$. So if $\overline{\Xi}$ is a resolution of $j_*p_Y^*(\overline{\eta})$ on W, then the restriction of $\overline{\Xi}$ to X (resp. P) provides a resolution of $i_*\overline{\eta}$ (resp. $i_{\infty *}\overline{\eta}$). The following theorem is the kernel of the whole proof of the vanishing theorem.

Theorem 3.18. *(Deformation theorem) Let $\overline{\Xi}$ be a resolution of $j_*p_Y^*(\overline{\eta})$ on W which satisfies the condition (T), then we have $\delta(\overline{\Xi}\mid_X)=\delta(\overline{\Xi}\mid_P)$.*

Proof. Consider the following tensor product of $\overline{\Xi}_\nabla\mid_{W(i_g)}$ with the Koszul resolution associated to the immersion $X_g\hookrightarrow W(i_g)$

$$0\to\overline{\Xi}_\nabla\mid_{W(i_g)}\otimes\overline{\mathcal{O}}(-X_g)\to\overline{\Xi}_\nabla\mid_{W(i_g)}\otimes\overline{\mathcal{O}}_{W(i_g)}\to\overline{\Xi}_\nabla\mid_{W(i_g)}\otimes i_{X_g*}\overline{\mathcal{O}}_{X_g}\to 0.$$

We have to caution the reader that here the tensor product is not the usual tensor product of two complexes, precisely our resulting sequence is a double complex and we don't take its total complex. Since we have assumed that $\overline{\Xi}$ satisfies the condition (T), this tensor product induces a short exact sequence of equivariant standard complexes on S by taking direct images. For $j\geq 0$, its j-th row is the following short exact sequence

$$\overline{\varepsilon}_j: 0\to R^0l_{g*}^0(\overline{\mathcal{O}}(-X_g)\otimes\overline{\overline{\widetilde{\xi}}}_j\mid_{W(i_g)})\to R^0l_{g*}^0(\overline{\overline{\widetilde{\xi}}}_j\mid_{W(i_g)})\to R^0h_{g*}(\overline{\overline{\widetilde{\xi}}}_j\mid_{X_g})\to 0$$

where l_g^0 is the composition of the inclusion $W(i_g)\hookrightarrow W$ with the morphism l. Note that the j-th homology of $\overline{\Xi}_\nabla\mid_{W(i_g)}$ is equal to $j_{g*}(\wedge^j\overline{\overline{\widetilde{F}}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mid_{W(i_g)}$ where $\widetilde{F}$ is the non-zero degree part of the normal bundle associated to the immersion j. Actually j_g factors through $j_g^0 : Y_g \times \mathbb{P}^1 \hookrightarrow W(i_g)$, then the j-th homology of $\overline{\Xi}_\nabla \mid_{W(i_g)}$ can be rewritten as $j^0_{g*}(\wedge^j \overline{\widetilde{F}}^\vee \otimes p^*_{Y_g}\overline{\eta} \mid_{Y_g})$. Write $Y_{g,0} := Y_g \times \{0\}$ for simplicity. Using the fact that $j_g^{0*}\mathcal{O}(-X_g)$ is isomorphic to $\mathcal{O}(-Y_{g,0})$, we deduce from the short exact sequence

$$0 \to j^0_{g*}(\overline{\mathcal{O}}(-Y_{g,0}) \otimes \wedge^j \overline{\widetilde{F}}^\vee \otimes p^*_{Y_g}\overline{\eta} \mid_{Y_g}) \to j^0_{g*}(\overline{\mathcal{O}}_{Y_g\times\mathbb{P}^1} \otimes \wedge^j \overline{\widetilde{F}}^\vee \otimes p^*_{Y_g}\overline{\eta} \mid_{Y_g})$$
$$\to j^0_{g*}(i_{Y_g*}\overline{\mathcal{O}}_{Y_g} \otimes \wedge^j \overline{\widetilde{F}}^\vee \otimes p^*_{Y_g}\overline{\eta} \mid_{Y_g}) \to 0$$

that the j-th homologies of the induced short exact sequence of equivariant standard complexes form a short exact sequence

$$\overline{\chi}_j : 0 \to R^0 u_{g*}(\overline{\mathcal{O}}(-Y_{g,0}) \otimes \wedge^j \overline{\widetilde{F}}^\vee \otimes p^*_{Y_g}\overline{\eta} \mid_{Y_g}) \to R^0 u_{g*}(\wedge^j \overline{\widetilde{F}}^\vee \otimes p^*_{Y_g}\overline{\eta} \mid_{Y_g})$$
$$\to R^0 f_{g*}(\wedge^j \overline{F}^\vee \otimes \overline{\eta} \mid_{Y_g}) \to 0$$

where u_g is the composition of the inclusion $Y_g \times \mathbb{P}^1 \hookrightarrow W(i_g)$ with the morphism l_g^0.
The main idea of this proof is that the equivariant Bott-Chern secondary characteristic class of the quotient term of the induced short exact sequence of equivariant standard complexes is nothing but $\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla \mid_X, h^H)$ which appears in the expression of $\delta(\overline{\Xi} \mid_X)$ and the equivariant secondary characteristic classes of $\overline{\chi}_j, \overline{\varepsilon}_j$ can be computed by Bismut-Ma's immersion formula.
Precisely, denote by g_{X_g} the Euler-Green current associated to X_g which was constructed by Bismut, Gillet and Soulé in [6, Section 3. (f)], it satisfies the differential equation $\mathrm{dd}^c g_{X_g} = \delta_{X_g} - c_1(\overline{\mathcal{O}}(X_g))$. We write $\mathrm{Td}(\overline{X_g})$ for $\mathrm{Td}(\overline{\mathcal{O}}(X_g))$, [6, Theorem 3.17] implies that $\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}$ is equal to the singular Bott-Chern current of the Koszul resolution associated to $X_g \hookrightarrow W(i_g)$ modulo $\mathrm{Im}\partial + \mathrm{Im}\overline{\partial}$. Moreover, write $\overline{\xi.}$ for the restriction $\overline{\Xi}_\nabla \mid_X$. Then for any $j \geq 0$, we compute

$$\begin{aligned}\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j) =& T_g(\omega^{X_g}, h^{\xi_j|_{X_g}}) - T_g(\omega^{W(i_g)}, h^{\widetilde{\xi}_j|_{W(i_g)}}) \\ &+ T_g(\omega^{W(i_g)}, h^{\mathcal{O}(-X_g)\otimes\widetilde{\xi}_j|_{W(i_g)}}) \\ &+ \int_{W(i_g)/S} \mathrm{ch}_g(\overline{\widetilde{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{X_g})g_{X_g} \\ &+ \int_{X_g/S} \mathrm{ch}_g(\overline{\xi}_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\widetilde{\mathrm{Td}}(\overline{Th_g}, \overline{Tl_g^0} \mid_{X_g}) \\ &+ \int_{X_g/S} \mathrm{ch}_g(\xi_j)R(N_{W(i_g)/X_g})\mathrm{Td}(Th_g).\end{aligned}$$

Here, one should note that to simplify the last two terms in the right-hand side of Bismut-Ma's immersion formula, we have used an Atiyah-Segal-Singer type formula for immersion

$$i_{g*}(\mathrm{Td}_g^{-1}(N)\mathrm{ch}_g(x)) = \mathrm{ch}_g(i_*(x)).$$

This formula is the content of [21, Theorem 6.16]. Similarly, for any $j \geq 0$, we compute

$$\begin{aligned}
\widetilde{\mathrm{ch}}_g(\overline{\chi}_j) =& T_g(\omega^{Y_g}, h^{\wedge^j F^\vee \otimes \eta|_{Y_g}}) - T_g(\omega^{Y_g \times \mathbb{P}^1}, h^{\wedge^j \widetilde{F}^\vee \otimes p_{Y_g}^* \eta|_{Y_g}}) \\
&+ T_g(\omega^{Y_g \times \mathbb{P}^1}, h^{\mathcal{O}(-Y_{g,0}) \otimes \wedge^j \widetilde{F}^\vee \otimes p_{Y_g}^* \eta|_{Y_g}}) \\
&+ \int_{Y_g \times \mathbb{P}^1/S} \mathrm{ch}_g(\wedge^j \overline{\widetilde{F}}^\vee \otimes p_{Y_g}^* \overline{\eta} \mid_{Y_g}) \mathrm{Td}(\overline{Tu_g}) \mathrm{Td}^{-1}(\overline{Y_{g,0}}) g_{Y_{g,0}} \\
&+ \int_{Y_g/S} \mathrm{ch}_g(\wedge^j \overline{F}^\vee \otimes \overline{\eta} \mid_{Y_g}) \mathrm{Td}^{-1}(\overline{N}_{Y_g \times \mathbb{P}^1/Y_{g,0}}) \widetilde{\mathrm{Td}}(\overline{Tf_g}, \overline{Tu_g} \mid_{Y_{g,0}}) \\
&+ \int_{Y_g/S} \mathrm{ch}_g(\wedge^j F^\vee \otimes \eta \mid_{Y_g}) R(N_{Y_g \times \mathbb{P}^1/Y_{g,0}}) \mathrm{Td}(Tf_g).
\end{aligned}$$

Denote by $\overline{\Omega}(W(i_g))$ (resp. $\overline{\Omega}(-X_g)$) the middle (resp. sub) term of the induced short exact sequence of equivariant standard complexes. According to Lemma 3.12, we have

$$\begin{aligned}
&\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla \mid_X, h^H) - \widetilde{\mathrm{ch}}_g(\overline{\Omega}(W(i_g)), h^H) + \widetilde{\mathrm{ch}}_g(\overline{\Omega}(-X_g), h^H) \\
=& \sum (-1)^j \widetilde{\mathrm{ch}}_g(\overline{\chi}_j) - \sum (-1)^j \widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j) \\
=& \sum (-1)^j T_g(\omega^{Y_g}, h^{\wedge^j F^\vee \otimes \eta|_{Y_g}}) - \sum (-1)^j T_g(\omega^{Y_g \times \mathbb{P}^1}, h^{\wedge^j \widetilde{F}^\vee \otimes p_{Y_g}^* \eta|_{Y_g}}) \\
&+ \sum (-1)^j T_g(\omega^{Y_g \times \mathbb{P}^1}, h^{\mathcal{O}(-Y_{g,0}) \otimes \wedge^j \widetilde{F}^\vee \otimes p_{Y_g}^* \eta|_{Y_g}}) \\
&+ \int_{Y_g \times \mathbb{P}^1/S} \sum (-1)^j \mathrm{ch}_g(\wedge^j \overline{\widetilde{F}}^\vee \otimes p_{Y_g}^* \overline{\eta} \mid_{Y_g}) \mathrm{Td}(\overline{Tu_g}) \mathrm{Td}^{-1}(\overline{Y_{g,0}}) g_{Y_{g,0}} \\
&+ \int_{Y_g/S} \sum (-1)^j \mathrm{ch}_g(\wedge^j \overline{F}^\vee \otimes \overline{\eta} \mid_{Y_g}) \mathrm{Td}^{-1}(\overline{N}_{Y_g \times \mathbb{P}^1/Y_{g,0}}) \widetilde{\mathrm{Td}}(\overline{Tf_g}, \overline{Tu_g} \mid_{Y_{g,0}}) \\
&+ \int_{Y_g/S} \sum (-1)^j \mathrm{ch}_g(\wedge^j F^\vee \otimes \eta \mid_{Y_g}) R(N_{Y_g \times \mathbb{P}^1/Y_{g,0}}) \mathrm{Td}(Tf_g) \\
&- \sum (-1)^j T_g(\omega^{X_g}, h^{\xi_j|_{X_g}}) + \sum (-1)^j T_g(\omega^{W(i_g)}, h^{\widetilde{\xi}_j|_{W(i_g)}}) \\
&- \sum (-1)^j T_g(\omega^{W(i_g)}, h^{\mathcal{O}(-X_g) \otimes \widetilde{\xi}_j|_{W(i_g)}}) \\
&- \int_{W(i_g)/S} \sum (-1)^j \mathrm{ch}_g(\overline{\widetilde{\xi}}_j) \mathrm{Td}(\overline{Tl_g^0}) \mathrm{Td}^{-1}(\overline{X_g}) g_{X_g} \\
&- \int_{X_g/S} \sum (-1)^j \mathrm{ch}_g(\overline{\xi}_j) \mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g}) \widetilde{\mathrm{Td}}(\overline{Th_g}, \overline{Tl_g^0} \mid_{X_g}) \\
&- \int_{X_g/S} \sum (-1)^j \mathrm{ch}_g(\xi_j) R(N_{W(i_g)/X_g}) \mathrm{Td}(Th_g). \qquad (1)
\end{aligned}$$

Similarly, we consider the tensor products of $\overline{\Xi}_\nabla \mid_{W(i_g)}$ with the following three Koszul resolutions

$$0 \to \overline{\mathcal{O}}(-P_g^0) \to \overline{\mathcal{O}}_{W(i_g)} \to i_{P_g^0 *} \overline{\mathcal{O}}_{P_g^0} \to 0,$$

$$0 \to \overline{\mathcal{O}}(-\widetilde{X_g}) \to \overline{\mathcal{O}}_{W(i_g)} \to i_{\widetilde{X_g}*}\overline{\mathcal{O}}_{\widetilde{X_g}} \to 0,$$

and

$$0 \to \overline{\mathcal{O}}(-\widetilde{X_g}) \otimes \overline{\mathcal{O}}(-P_g^0) \to \overline{\mathcal{O}}(-\widetilde{X_g}) \oplus \overline{\mathcal{O}}(-P_g^0) \to \overline{\mathcal{O}}_{W(i_g)} \to i_{\widetilde{X_g}\cap P_g^0 *}\overline{\mathcal{O}}_{\widetilde{X_g}\cap P_g^0} \to 0.$$

We shall still denote by $\overline{\chi.}$ (resp. $\overline{\varepsilon.}$) the exact sequences consisting of homologies (resp. elements) in the induced exact sequences of equivariant standard complexes.

For the first one, denote by $g_{P_g^0}$ the Euler-Green current associated to P_g^0 and write $\overline{\xi.}^{\infty}$ for the restriction $\overline{\Xi}_\nabla\mid_P$. Moreover, denote by $\overline{\Omega}(-P_g^0)$ the sub term of the induced short exact sequence of equivariant standard complexes and denote by b_g the composition of the inclusion $P_g^0 \hookrightarrow W(i_g)$ with the morphism l_g^0. According to Lemma 3.12, we have

$$\begin{aligned}
&\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_{P_g^0}, h^H) - \widetilde{\mathrm{ch}}_g(\overline{\Omega}(W(i_g)), h^H) + \widetilde{\mathrm{ch}}_g(\overline{\Omega}(-P_g^0), h^H)\\
=&\sum(-1)^j\widetilde{\mathrm{ch}}_g(\overline{\chi}_j) - \sum(-1)^j\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j)\\
=&\sum(-1)^jT_g(\omega^{Y_g}, h^{\wedge^j F_\infty^\vee\otimes\eta|_{Y_g}}) - \sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1}, h^{\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})\\
&+\sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1}, h^{\mathcal{O}(-Y_{g,\infty})\otimes\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})\\
&+\int_{Y_g\times\mathbb{P}^1/S}\sum(-1)^j\mathrm{ch}_g(\wedge^j\overline{\widetilde{F}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mathrm{Td}(\overline{Tu_g})\mathrm{Td}^{-1}(\overline{Y_{g,\infty}})g_{Y_{g,\infty}}\\
&+\int_{Y_g/S}\{\sum(-1)^j\mathrm{ch}_g(\wedge^j\overline{F}_\infty^\vee\otimes\overline{\eta}\mid_{Y_g})\mathrm{Td}^{-1}(\overline{N}_{Y_g\times\mathbb{P}^1/Y_{g,\infty}})\\
&\qquad\qquad\cdot\widetilde{\mathrm{Td}}(\overline{Tf_g}, \overline{Tu_g}\mid_{Y_{g,\infty}})\}\\
&+\int_{Y_g/S}\sum(-1)^j\mathrm{ch}_g(\wedge^jF_\infty^\vee\otimes\eta\mid_{Y_g})R(N_{Y_g\times\mathbb{P}^1/Y_{g,\infty}})\mathrm{Td}(Tf_g)\\
&-\sum(-1)^jT_g(\omega^{P_g^0}, h^{\xi_j^\infty|_{P_g^0}}) + \sum(-1)^jT_g(\omega^{W(i_g)}, h^{\widetilde{\xi}_j|_{W(i_g)}})\\
&-\sum(-1)^jT_g(\omega^{W(i_g)}, h^{\mathcal{O}(-P_g^0)\otimes\widetilde{\xi}_j|_{W(i_g)}})\\
&-\int_{W(i_g)/S}\sum(-1)^j\mathrm{ch}_g(\overline{\widetilde{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}\\
&-\int_{P_g^0/S}\sum(-1)^j\mathrm{ch}_g(\overline{\xi}_j^\infty)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P_g^0})\widetilde{\mathrm{Td}}(\overline{Tb_g}, \overline{Tl_g^0}\mid_{P_g^0})\\
&-\int_{P_g^0/S}\sum(-1)^j\mathrm{ch}_g(\xi_j^\infty)R(N_{W(i_g)/P_g^0})\mathrm{Td}(Tb_g) \qquad (2)
\end{aligned}$$

where $\overline{F}_\infty$ is the non-zero degree part of the hermitian normal bundle $\overline{N}_\infty$ associated to i_∞.

For the second one, denote by $g_{\widetilde{X_g}}$ the Euler-Green current associated to $\widetilde{X_g}$ and denote by $\overline{\Omega}(-\widetilde{X_g})$ the sub term of the induced short exact sequence of equivariant standard complexes. Since the restriction of $\overline{\Xi}$ to the component $\widetilde{X}$ is equivariantly and orthogonally split, we know that $\widetilde{\mathrm{ch}}_g(\Xi\mid_{\widetilde{X_g}},h^H)$ is equal to 0 and the summation $\sum(-1)^j\mathrm{ch}_g(\overline{\widetilde{\xi}}_j)$ vanishes on $\widetilde{X_g}$. Using again Lemma 3.12, we obtain

$$\begin{aligned}
&-\widetilde{\mathrm{ch}}_g(\overline{\Omega}(W(i_g)),h^H)+\widetilde{\mathrm{ch}}_g(\overline{\Omega}(-\widetilde{X_g}),h^H)\\
=&\sum(-1)^j\widetilde{\mathrm{ch}}_g(\overline{\chi}_j)-\sum(-1)^j\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j)\\
=&-\sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1},h^{\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})\\
&+\sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1},h^{j_g^{0*}\mathcal{O}(-\widetilde{X_g})\otimes\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})\\
&-\int_{Y_g\times\mathbb{P}^1/S}\{\sum(-1)^j\mathrm{ch}_g(\wedge^j\overline{\widetilde{F}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mathrm{Td}(\overline{Tu_g})\\
&\qquad\qquad\cdot\widetilde{\mathrm{ch}}(j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X_g}),\overline{O}_{Y_g\times\mathbb{P}^1})\}\\
&+\sum(-1)^jT_g(\omega^{W(i_g)},h^{\widetilde{\xi}_j|_{W(i_g)}})\\
&-\sum(-1)^jT_g(\omega^{W(i_g)},h^{\mathcal{O}(-\widetilde{X_g})\otimes\widetilde{\xi}_j|_{W(i_g)}})\\
&-\int_{W(i_g)/S}\sum(-1)^j\mathrm{ch}_g(\overline{\widetilde{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}}. \qquad (3)
\end{aligned}$$

Here the element $\widetilde{\mathrm{ch}}(j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X_g}),\overline{O}_{Y_g\times\mathbb{P}^1})$ is the equivariant secondary characteristic class of the following short exact sequence

$$0\to 0\to j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X_g})\to\overline{O}_{Y_g\times\mathbb{P}^1}\to 0.$$

We now consider the last one. This is also a Koszul resolution because $\widetilde{X_g}$ and P_g^0 intersect transversally. By [6, Theorem 3.20], the Euler-Green current associated to $\widetilde{X_g}\cap P_g^0$ is the current $c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}+\delta_{\widetilde{X_g}}g_{P_g^0}$. Then, by using the isometry $\overline{\mathcal{O}}(X_g)\cong\overline{\mathcal{O}}(P_g^0)\otimes\overline{\mathcal{O}}(\widetilde{X_g})$ and Corollary 3.13, we get

$$\begin{aligned}
&-\widetilde{\mathrm{ch}}_g(\overline{\Omega}(W(i_g)),h^H)+\widetilde{\mathrm{ch}}_g(\overline{\Omega}(-\widetilde{X_g}),h^H)\\
&\qquad\qquad+\widetilde{\mathrm{ch}}_g(\overline{\Omega}(-P_g^0),h^H)-\widetilde{\mathrm{ch}}_g(\overline{\Omega}(-X_g),h^H)\\
=&\sum(-1)^j\widetilde{\mathrm{ch}}_g(\overline{\chi}_j)-\sum(-1)^j\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}_j)\\
=&-\sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1},h^{\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})\\
&+\sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1},h^{j_g^{0*}\mathcal{O}(-\widetilde{X_g})\otimes\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})\\
&+\sum(-1)^jT_g(\omega^{Y_g\times\mathbb{P}^1},h^{\mathcal{O}(-Y_{g,\infty})\otimes\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}})
\end{aligned}$$

$$
\begin{aligned}
&- \sum(-1)^j T_g(\omega^{Y_g\times\mathbb{P}^1}, h^{\mathcal{O}(-Y_{g,0})\otimes\wedge^j\widetilde{F}^\vee\otimes p_{Y_g}^*\eta|_{Y_g}}) \\
&- \int_{Y_g\times\mathbb{P}^1/S}\sum(-1)^j \mathrm{ch}_g(\wedge^j\overline{\widetilde{F}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mathrm{Td}(\overline{Tu_g})\widetilde{\mathrm{ch}}(\overline{\Theta}) \\
&+ \sum(-1)^j T_g(\omega^{W(i_g)}, h^{\widetilde{\xi}_j|_{W(i_g)}}) \\
&- \sum(-1)^j T_g(\omega^{W(i_g)}, h^{\mathcal{O}(-\widetilde{X}_g)\otimes\widetilde{\xi}_j|_{W(i_g)}}) \\
&- \sum(-1)^j T_g(\omega^{W(i_g)}, h^{\mathcal{O}(-P_g^0)\otimes\widetilde{\xi}_j|_{W(i_g)}}) \\
&+ \sum(-1)^j T_g(\omega^{W(i_g)}, h^{\mathcal{O}(-X_g)\otimes\widetilde{\xi}_j|_{W(i_g)}}) \\
&- \int_{W(i_g)/S}\{\sum(-1)^j \mathrm{ch}_g(\overline{\widetilde{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{\widetilde{X}_g})\mathrm{Td}^{-1}(\overline{P_g^0}) \\
&\qquad\qquad \cdot[c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X}_g}+\delta_{\widetilde{X}_g}g_{P_g^0}]\}.
\end{aligned}
\tag{4}
$$

Here the element $\widetilde{\mathrm{ch}}(\overline{\Theta})$ is the equivariant secondary characteristic class of the following short exact sequence

$$\overline{\Theta}:\quad 0\to\overline{\mathcal{O}}(-Y_{g,0})\to j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X}_g)\oplus\overline{\mathcal{O}}(-Y_{g,\infty})\to\overline{O}_{Y_g\times\mathbb{P}^1}\to 0.$$

Since $s_0: Y\times\{0\}\to Y\times\mathbb{P}^1$ and $s_\infty: Y\times\{\infty\}\to Y\times\mathbb{P}^1$ are sections of smooth morphism, the normal sequences

$$0\to\overline{Tf_g}\to\overline{Tu_g}\mid_{Y_{g,0}}\to\overline{N}_{Y_g\times\mathbb{P}^1/Y_{g,0}}\to 0$$

and

$$0\to\overline{Tf_g}\to\overline{Tu_g}\mid_{Y_{g,\infty}}\to\overline{N}_{Y_g\times\mathbb{P}^1/Y_{g,\infty}}\to 0$$

are orthogonally split so that $\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tu_g}\mid_{Y_{g,0}})$ and $\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tu_g}\mid_{Y_{g,\infty}})$ are both equal to 0. Moreover, the normal bundles $N_{Y_g\times\mathbb{P}^1/Y_{g,0}}$ and $N_{Y_g\times\mathbb{P}^1/Y_{g,\infty}}$ are isomorphic to trivial bundles so that $R(N_{Y_g\times\mathbb{P}^1/Y_{g,0}})$ and $R(N_{Y_g\times\mathbb{P}^1/Y_{g,\infty}})$ are both equal to 0. Furthermore, we may drop all the terms where an integral is taken over $\widetilde{X}_g$ because $\sum(-1)^j\mathrm{ch}_g(\overline{\widetilde{\xi}}_j)$ vanishes on $\widetilde{X}_g$.

Now, we compute (1)−(2)−(3)+(4) which is

$$
\begin{aligned}
&\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_X, h^H)-\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_{P_g^0}, h^H)+\sum(-1)^j T_g(\omega^{X_g}, h^{\xi_j|_{X_g}}) \\
&\quad -\sum(-1)^j T_g(\omega^{P_g^0}, h^{\xi_j^\infty|_{P_g^0}})-\sum(-1)^j T_g(\omega^{Y_g}, h^{\wedge^j F^\vee\otimes\eta|_{Y_g}}) \\
&\qquad\qquad +\sum(-1)^j T_g(\omega^{Y_g}, h^{\wedge^j F_\infty^\vee\otimes\eta|_{Y_g}}) \\
&=\int_{Y_g\times\mathbb{P}^1/S}\{\sum(-1)^j\mathrm{ch}_g(\wedge^j\overline{\widetilde{F}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mathrm{Td}(\overline{Tu_g})\cdot[\mathrm{Td}^{-1}(\overline{Y_{g,0}})g_{Y_{g,0}} \\
&\qquad -\mathrm{Td}^{-1}(\overline{Y_{g,\infty}})g_{Y_{g,\infty}}+\widetilde{\mathrm{ch}}(j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X}_g),\overline{O}_{Y_g\times\mathbb{P}^1})-\widetilde{\mathrm{ch}}_g(\overline{\Theta})]\}
\end{aligned}
$$

$$
\begin{aligned}
&-\int_{W(i_g)/S}\sum(-1)^j\mathrm{ch}_g(\overline{\overline{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}\\
&-\int_{X_g/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl_g^0}\mid_{X_g})\\
&-\int_{X_g/S}\sum(-1)^j\mathrm{ch}_g(\xi_j)R(N_{W(i_g)/X_g})\mathrm{Td}(Th_g)\\
&+\int_{W(i_g)/S}\sum(-1)^j\mathrm{ch}_g(\overline{\overline{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}\\
&+\int_{P_g^0/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}_j^{\infty})\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P_g^0})\widetilde{\mathrm{Td}}(\overline{Tb_g},\overline{Tl_g^0}\mid_{P_g^0})\\
&+\int_{P_g^0/S}\sum(-1)^j\mathrm{ch}_g(\xi_j^{\infty})R(N_{W(i_g)/P_g^0})\mathrm{Td}(Tb_g)\\
&+\int_{W(i_g)/S}\sum(-1)^j\mathrm{ch}_g(\overline{\overline{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{\widetilde{X}_g})g_{\widetilde{X}_g}\\
&-\int_{W(i_g)/S}\sum(-1)^j\mathrm{ch}_g(\overline{\overline{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\mathrm{Td}^{-1}(\overline{\widetilde{X}_g})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X}_g}.
\end{aligned}
$$

Denote by i_X (resp. i_P) the inclusion from X to $W(i)$ (resp. P to $W(i)$). We may use the Atiyah-Segal-Singer type formula for immersions and the projection formula in cohomology to compute

$$
\begin{aligned}
&i_{X_g*}\big(\sum(-1)^j\mathrm{ch}_g(\xi_j)R(N_{W(i_g)/X_g})\mathrm{Td}(Th_g)\big)\\
=&i_{X_g*}\big(R(N_{W(i_g)/X_g})\mathrm{Td}(Th_g)i_{g*}(\mathrm{Td}_g^{-1}(N_{X/Y})\mathrm{ch}_g(\eta))\big)\\
=&(i_{X_g}\circ i_g)_*\big(R(N_{W(i_g)/X_g})\mathrm{Td}(Th_g)\mathrm{Td}_g^{-1}(N_{X/Y})\mathrm{ch}_g(\eta)\big).
\end{aligned}
$$

Note that the restriction of $N_{W(i_g)/X_g}$ to Y_g is trivial so that the last expression vanishes. An entirely analogous reasoning implies that

$$
i_{P_g*}\big(\sum(-1)^j\mathrm{ch}_g(\xi_j^{\infty})R(N_{W(i_g)/P_g^0})\mathrm{Td}(Tb_g)\big)=0.
$$

Thus, we are left with the equality

$$
\begin{aligned}
&\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_X,h^H)-\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_{P_g^0},h^H)+\sum(-1)^jT_g(\omega^{X_g},h^{\xi_j\mid_{X_g}})\\
&-\sum(-1)^jT_g(\omega^{P_g^0},h^{\xi_j^{\infty}\mid_{P_g^0}})-\sum(-1)^jT_g(\omega^{Y_g},h^{\wedge^jF^\vee\otimes\eta\mid_{Y_g}})\\
&\qquad\qquad+\sum(-1)^jT_g(\omega^{Y_g},h^{\wedge^jF_\infty^\vee\otimes\eta\mid_{Y_g}})\\
=&\int_{Y_g\times\mathbb{P}^1/S}\{\sum(-1)^j\mathrm{ch}_g(\wedge^j\overline{\widetilde{F}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mathrm{Td}(\overline{Tu_g})\cdot[\mathrm{Td}^{-1}(\overline{Y_{g,0}})g_{Y_{g,0}}\\
&\qquad-\mathrm{Td}^{-1}(\overline{Y_{g,\infty}})g_{Y_{g,\infty}}+\widetilde{\mathrm{ch}}(j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X}_g),\overline{O_{Y_g\times\mathbb{P}^1}})-\widetilde{\mathrm{ch}}_g(\overline{\Theta})]\}\\
&-\int_{W(i_g)/S}\{\sum(-1)^j\mathrm{ch}_g(\overline{\overline{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\cdot[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}-\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}
\end{aligned}
$$

$$- \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}} + \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}$$
$$- \int_{X_g/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl_g^0}\mid_{X_g})$$
$$+ \int_{P_g^0/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}_j^\infty)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P_g^0})\widetilde{\mathrm{Td}}(\overline{Tb_g},\overline{Tl_g^0}\mid_{P_g^0}).$$

Using the differential equation which $T_g(\overline{\widetilde{\xi}}.)$ satisfies, we compute

$$\begin{aligned}
&- \int_{W(i_g)/S}\{\sum(-1)^j\mathrm{ch}_g(\overline{\widetilde{\xi}}_j)\mathrm{Td}(\overline{Tl_g^0})\cdot[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g} - \mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}\\
&\qquad - \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}} + \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}\\
&= \int_{W(i_g)/S}\{\mathrm{Td}(\overline{Tl_g^0})T_g(\overline{\widetilde{\xi}}.)\cdot[\mathrm{Td}^{-1}(\overline{X_g})\delta_{X_g} - \mathrm{Td}^{-1}(\overline{P_g^0})\delta_{P_g^0}\\
&\qquad - \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\delta_{\widetilde{X_g}} + \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))\delta_{\widetilde{X_g}}]\}\\
&- \int_{W(i_g)/S}\{\mathrm{Td}(\overline{Tl_g^0})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_{W/Y\times\mathbb{P}^1})\delta_{Y_g\times\mathbb{P}^1}\cdot[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}\\
&- \mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0} - \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}} + \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}.
\end{aligned} \tag{5}$$

Here we have used the equation

$$\begin{aligned}
\mathrm{Td}^{-1}(\overline{X_g})c_1(\overline{\mathcal{O}}(X_g)) - \mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0)) - \mathrm{Td}^{-1}(\overline{\widetilde{X_g}})c_1(\overline{\mathcal{O}}(\widetilde{X_g}))\\
+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))c_1(\overline{\mathcal{O}}(\widetilde{X_g})) = 0
\end{aligned} \tag{6}$$

which is [21, (23)].

Again using the fact that $\overline{\widetilde{\xi}}.$ is equivariantly and orthogonally split on $\widetilde{X}$, the first integral in the right-hand side of (5) is equal to

$$\int_{X_g/S}\mathrm{Td}(\overline{Tl_g^0})T_g(\overline{\xi}.)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g}) - \int_{P_g^0/S}\mathrm{Td}(\overline{Tl_g^0})T_g(\overline{\xi.}^\infty)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P_g^0}).$$

According to the normal sequence $0 \to \overline{Th_g} \to \overline{Tl_g^0}\mid_{X_g} \to \overline{N}_{W(i_g)/X_g} \to 0$, we may write

$$\mathrm{Td}(\overline{Tl_g^0}) = \mathrm{Td}(\overline{Th_g})\mathrm{Td}(\overline{N}_{W(i_g)/X_g}) - \mathrm{dd}^c\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl_g^0}\mid_{X_g}).$$

So we get

$$\begin{aligned}
&\int_{X_g/S}\mathrm{Td}(\overline{Tl^0_g})T_g(\overline{\xi.})\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\\
=&\int_{X_g/S}\mathrm{Td}(\overline{Th_g})T_g(\overline{\xi.})\\
&-\int_{X_g/S}\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl^0_g}\mid_{X_g})\delta_{Y_g}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\\
&+\int_{X_g/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl^0_g}\mid_{X_g}).
\end{aligned}$$

Similarly we have

$$\begin{aligned}
&\int_{P^0_g/S}\mathrm{Td}(\overline{Tl^0_g})T_g(\overline{\xi.}^\infty)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P^0_g})\\
=&\int_{P^0_g/S}\mathrm{Td}(\overline{Tb_g})T_g(\overline{\xi.}^\infty)\\
&-\int_{P^0_g/S}\widetilde{\mathrm{Td}}(\overline{Tb_g},\overline{Tl^0_g}\mid_{P^0_g})\delta_{Y_g}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_\infty)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P^0_g})\\
&+\int_{P^0_g/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}^\infty_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P^0_g})\widetilde{\mathrm{Td}}(\overline{Tb_g},\overline{Tl^0_g}\mid_{P^0_g}).
\end{aligned}$$

Note that the normal sequence of $\overline{Th_g}$ in $\overline{Tl^0_g}$ (resp. $\overline{Tb_g}$ in $\overline{Tl^0_g}$) is orthogonally split on $Y_g\times\{0\}$ (resp. $Y_g\times\{\infty\}$), then $\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl^0_g}\mid_{X_g})\delta_{Y_g}$ and $\widetilde{\mathrm{Td}}(\overline{Tb_g},\overline{Tl^0_g}\mid_{P^0_g})\delta_{Y_g}$ are both equal to 0. Combining these computations above we get

$$\begin{aligned}
&\int_{X_g/S}\mathrm{Td}(\overline{Tl^0_g})T_g(\overline{\xi.})\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\\
&\qquad\qquad-\int_{P^0_g/S}\mathrm{Td}(\overline{Tl^0_g})T_g(\overline{\xi.}^\infty)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P^0_g})\\
=&\int_{X_g/S}\mathrm{Td}(\overline{Th_g})T_g(\overline{\xi.})\\
&+\int_{X_g/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/X_g})\widetilde{\mathrm{Td}}(\overline{Th_g},\overline{Tl^0_g}\mid_{X_g})\\
&-\int_{P^0_g/S}\mathrm{Td}(\overline{Tb_g})T_g(\overline{\xi.}^\infty)\\
&-\int_{P^0_g/S}\sum(-1)^j\mathrm{ch_g}(\overline{\xi}^\infty_j)\mathrm{Td}^{-1}(\overline{N}_{W(i_g)/P^0_g})\widetilde{\mathrm{Td}}(\overline{Tb_g},\overline{Tl^0_g}\mid_{P^0_g}).
\end{aligned}\tag{7}$$

We now compute the second integral in the right-hand side of (5). According to the normal sequence

$$0\to\overline{Tu_g}\to\overline{Tl_g^0}\mid_{Y_g\times\mathbb{P}^1}\to\overline{N}_{W(i_g)/Y_g\times\mathbb{P}^1}\to 0,$$

we may write

$$\mathrm{Td}(\overline{Tl_g^0})=\mathrm{Td}(\overline{Tu_g})\mathrm{Td}(\overline{N}_{W(i_g)/Y_g\times\mathbb{P}^1})-\mathrm{dd}^c\widetilde{\mathrm{Td}}(\overline{Tu_g},\overline{Tl_g^0}\mid_{Y_g\times\mathbb{P}^1}).$$

Hence

$$\begin{aligned}
&-\int_{W(i_g)/S}\{\mathrm{Td}(\overline{Tl_g^0})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_{W/Y\times\mathbb{P}^1})\delta_{Y_g\times\mathbb{P}^1}\cdot[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}\\
&-\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}-\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}}+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}\\
=&-\int_{Y_g\times\mathbb{P}^1/S}\{\mathrm{Td}(\overline{Tu_g})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{\overline{F}})\cdot j_g^{0*}[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}\\
&-\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}-\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}}+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}\\
&+\int_{Y_g\times\mathbb{P}^1/S}\{\widetilde{\mathrm{Td}}(\overline{Tu_g},\overline{Tl_g^0}\mid_{Y_g\times\mathbb{P}^1})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_{W/Y\times\mathbb{P}^1})\\
&\cdot[\mathrm{Td}^{-1}(\overline{X_g})(\delta_{X_g}-c_1(\overline{\mathcal{O}}(X_g)))-\mathrm{Td}^{-1}(\overline{P_g^0})(\delta_{P_g^0}-c_1(\overline{\mathcal{O}}(P_g^0)))\\
&-\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})(\delta_{\widetilde{X_g}}-c_1(\overline{\mathcal{O}}(\widetilde{X_g})))\\
&+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))(\delta_{\widetilde{X_g}}-c_1(\overline{\mathcal{O}}(\widetilde{X_g})))]\}.
\end{aligned}$$

By our choices of the metrics, we have $\mathrm{Td}_g^{-1}(\overline{N}_{W/Y\times\mathbb{P}^1})\mid_{Y_{g,0}}=\mathrm{Td}_g^{-1}(\overline{N})$, $\mathrm{Td}(\overline{X_g})\mid_{Y_{g,0}}=1$ and $\mathrm{Td}_g^{-1}(\overline{N}_{W/Y\times\mathbb{P}^1})\mid_{Y_{g,\infty}}=\mathrm{Td}_g^{-1}(\overline{N}_\infty)$, $\mathrm{Td}(\overline{P_g^0})\mid_{Y_{g,\infty}}=1$. Furthermore, by replacing all tangent bundles by relative tangent bundles, on can carry through the proof given in [21, P. 378-379] to show that

$$\widetilde{\mathrm{Td}}(\overline{Tu_g},\overline{Tl_g^0}\mid_{Y_g\times\mathbb{P}^1})\mid_{Y_{g,0}}=\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Th_g}\mid_{Y_g})$$

and

$$\widetilde{\mathrm{Td}}(\overline{Tu_g},\overline{Tl_g^0}\mid_{Y_g\times\mathbb{P}^1})\mid_{Y_{g,\infty}}=\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tb_g}\mid_{Y_g}).$$

So combining with the equation (6), we get

$$\begin{aligned}
&-\int_{W(i_g)/S}\{\mathrm{Td}(\overline{Tl_g^0})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_{W/Y\times\mathbb{P}^1})\delta_{Y_g\times\mathbb{P}^1}\cdot[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}\\
&-\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}-\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}}+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}\\
=&-\int_{Y_g\times\mathbb{P}^1/S}\{\mathrm{Td}(\overline{Tu_g})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{\overline{F}})\cdot j_g^{0*}[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}\\
&-\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}-\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}}+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}
\end{aligned}$$

$$+\int_{Y_g/S}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Th_g}\mid_{Y_g})$$
$$-\int_{Y_g/S}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_\infty)\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tb_g}\mid_{Y_g}). \tag{8}$$

At last, using the fact that the intersections in the deformation diagram are transversal and the fact that $j_g^0(Y_g\times\mathbb{P}^1)$ has no intersection with $\widetilde{X_g}$, we can compute

$$\int_{Y_g\times\mathbb{P}^1/S}\{\sum(-1)^j\mathrm{ch}_g(\wedge^j\overline{\widetilde{F}}^\vee\otimes p_{Y_g}^*\overline{\eta}\mid_{Y_g})\mathrm{Td}(\overline{Tu_g})\cdot[\mathrm{Td}^{-1}(\overline{Y_{g,0}})g_{Y_{g,0}}$$
$$-\mathrm{Td}^{-1}(\overline{Y_{g,\infty}})g_{Y_{g,\infty}}+\widetilde{\mathrm{ch}}(j_g^{0*}\overline{\mathcal{O}}(-\widetilde{X_g}),\overline{O}_{Y_g\times\mathbb{P}^1})-\widetilde{\mathrm{ch}}_g(\overline{\Theta})]\}$$
$$=\int_{Y_g\times\mathbb{P}^1/S}\{\mathrm{Td}(\overline{Tu_g})\mathrm{ch}_g(p_Y^*\overline{\eta})\mathrm{Td}_g^{-1}(\overline{\widetilde{F}})\cdot j_g^{0*}[\mathrm{Td}^{-1}(\overline{X_g})g_{X_g}-\mathrm{Td}^{-1}(\overline{P_g^0})g_{P_g^0}$$
$$-\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})g_{\widetilde{X_g}}+\mathrm{Td}^{-1}(\overline{\widetilde{X_g}})\mathrm{Td}^{-1}(\overline{P_g^0})c_1(\overline{\mathcal{O}}(P_g^0))g_{\widetilde{X_g}}]\}. \tag{9}$$

Gathering (5), (7), (8) and (9) we finally get

$$\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_X,h^H)-\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_{P_g^0},h^H)+\sum(-1)^jT_g(\omega^{X_g},h^{\xi_j\mid_{X_g}})$$
$$-\sum(-1)^jT_g(\omega^{P_g^0},h^{\xi_j^\infty\mid_{P_g^0}})-\sum(-1)^jT_g(\omega^{Y_g},h^{\wedge^jF^\vee\otimes\eta\mid_{Y_g}})$$
$$+\sum(-1)^jT_g(\omega^{Y_g},h^{\wedge^jF_\infty^\vee\otimes\eta\mid_{Y_g}})$$
$$=\int_{X_g/S}\mathrm{Td}(\overline{Th_g})T_g(\overline{\xi.})-\int_{P_g^0/S}\mathrm{Td}(\overline{Tb_g})T_g(\overline{\xi.}^\infty)$$
$$+\int_{Y_g/S}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Th_g}\mid_{Y_g})$$
$$-\int_{Y_g/S}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_\infty)\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tb_g}\mid_{Y_g}). \tag{10}$$

On the other hand, by definition, we have

$$\delta(\overline{\Xi}\mid_P):=\widetilde{\mathrm{ch}}_g(\overline{\xi.}^\infty,\overline{\eta})-\sum_k(-1)^kT_g(\omega^{Y_g},h^{\wedge^kF_\infty^\vee\otimes\eta\mid_{Y_g}})$$
$$+\sum_k(-1)^kT_g(\omega^{P_g},h^{\xi_k^\infty\mid_{P_g}})$$
$$-\int_{Y_g/S}\mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)$$
$$-\int_{P_g/S}T_g(\overline{\xi.}^\infty)\mathrm{Td}(\overline{Tb'_g})$$

$$-\int_{Y_g/S}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_\infty)\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tb'_g}\mid_{Y_g})$$

where $b' : P \to S$ is the composition of the inclusion $P \hookrightarrow W(i)$ and the morphism l. Note that P_g^0 is an open and closed submanifold of P_g and $\overline{\xi.}^\infty$ is orthogonally split on the other components since they all belong to $\widetilde{X}_g$, then we can rewrite $\delta(\overline{\Xi}\mid_P)$ as

$$\begin{aligned}\delta(\overline{\Xi}\mid_P) =&\widetilde{\mathrm{ch}}_g(\overline{\Xi}_\nabla\mid_{P_g^0},h^H)-\sum_k(-1)^kT_g(\omega^{Y_g},h^{\wedge^k F_\infty^\vee\otimes\eta|_{Y_g}})\\ &+\sum_k(-1)^kT_g(\omega^{P_g^0},h^{\xi_k^\infty|_{P_g^0}})\\ &-\int_{Y_g/S}\mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)\\ &-\int_{P_g^0/S}T_g(\overline{\xi.}^\infty)\mathrm{Td}(\overline{Tb_g})\\ &-\int_{Y_g/S}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N}_\infty)\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tb_g}\mid_{Y_g}).\end{aligned}$$

Comparing with the definition of $\delta(\overline{\Xi}\mid_X)$, the equality (10) implies that

$$\delta(\overline{\Xi}\mid_X)-\delta(\overline{\Xi}\mid_P)=0$$

which completes the proof of this deformation theorem. □

Now we consider the zero section imbedding $i_\infty : Y \to P = \mathbb{P}(N_\infty \oplus \mathcal{O}_Y)$. Here we use the fact that N_∞ is isomorphic to $N_{X/Y}$, we caution the reader that this is not necessarily an isometry since $\overline{N}_\infty$ carries the quotient metric induced by the Kähler metric on P but $N_{X/Y}$ carries the quotient metric induced by the Kähler metric on X. We recall that on P we have a tautological exact sequence

$$0\to\mathcal{O}(-1)\to\pi_P^*(N_\infty\oplus\mathcal{O}_Y)\to Q\to 0.$$

The equivariant section $\sigma : \mathcal{O}_P \to \pi_P^*(N_\infty \oplus \mathcal{O}_Y) \to Q$ induces the following Koszul resolution

$$0\to\wedge^{\mathrm{rk}Q}Q^\vee\to\cdots\to Q^\vee\to\mathcal{O}_P\to i_{\infty *}\mathcal{O}_Y\to 0.$$

Since σ is equivariant, the image of $\mathcal{O}_{P_g}$ under $\sigma\mid_{P_g}$ is contained in Q_g. This means that $\sigma\mid_{P_g}$ induces a Koszul resolution on P_g of the following form

$$0\to\wedge^{\mathrm{rk}Q_g}Q_g^\vee\to\cdots\to Q_g^\vee\to\mathcal{O}_{P_g}\to i_{\infty,g_*}\mathcal{O}_{Y_g}\to 0.$$

PROPOSITION 3.19. *Let $\overline{\kappa} := \overline{\kappa}(\overline{\eta}, \overline{N}_\infty)$ be a hermitian Koszul resolution on P defined in Definition 3.3. Then for $n \gg 0$, we have $\delta(\overline{\kappa}(n)) = 0$.*

Proof. Denote the non-zero degree part of $Q\mid_{P_g}$ by $Q_\perp$, then we have the following isometry

$$\wedge^i\overline{Q}^\vee\mid_{P_g}=\wedge^i(\overline{Q}_g^\vee\oplus\overline{Q}_\perp^\vee)\cong\bigoplus_{t+s=i}(\wedge^t\overline{Q}_g^\vee\otimes\wedge^s\overline{Q}_\perp^\vee).$$

Consider the following complex of equivariant hermitian vector bundles on P_g

$$\begin{aligned}0\to\wedge^{\mathrm{rk}Q_g}\overline{Q}_g^\vee\otimes(\wedge^k\overline{Q}_\perp^\vee\otimes\pi_{P_g}^*\overline{\eta}\mid_{Y_g})\to\cdots\to\overline{Q}_g^\vee\otimes(\wedge^k\overline{Q}_\perp^\vee\otimes\pi_{P_g}^*\overline{\eta}\mid_{Y_g})\\ \to\wedge^k\overline{Q}_\perp^\vee\otimes\pi_{P_g}^*\overline{\eta}\mid_{Y_g}\to 0\end{aligned}$$

which provides a resolution of $i_{\infty,g_*}(\wedge^k\overline{F}_\infty^\vee\otimes\overline{\eta}\mid_{Y_g})$ where F_∞, as before, is the non-zero degree part of the normal bundle N_∞ associated to i_∞. We denote this resolution by $\overline{\kappa}^{(k)}$, then according to the arguments given before this proposition we have a decomposition of complexes $\overline{\kappa}_\nabla\mid_{P_g}\cong\bigoplus_{k\geq 0}\overline{\kappa}_\nabla^{(k)}[-k]$ where $\overline{\kappa}_\nabla^{(k)}[-k]$ is obtained from $\overline{\kappa}_\nabla^{(k)}$ by shifting degree. Replacing $\overline{\kappa}$ by $\overline{\kappa}(n)$ for big enough n, we may assume that all elements in $\overline{\kappa}$ and $\overline{\kappa}^{(k)}$ are acyclic. Therefore, by Bisumt-Ma's immersion formula we have the following equality

$$\begin{aligned}\widetilde{\mathrm{ch}}_g(b'_{g_*}\overline{\kappa}^{(k)})=&T_g(\omega^{Y_g},h^{\wedge^kF_\infty^\vee\otimes\eta\mid_{Y_g}})-\sum_{i=0}^{\mathrm{rk}Q_g}(-1)^iT_g(\omega^{P_g},h^{\wedge^iQ_g^\vee\otimes\wedge^kQ_\perp^\vee\otimes\pi_{P_g}^*\eta\mid_{Y_g}})\\ &+\int_{Y_g/S}\mathrm{ch}_g(\wedge^kF_\infty^\vee\otimes\eta\mid_{Y_g})R(N_{\infty,g})\mathrm{Td}(Tf_g)\\ &+\int_{P_g/S}\mathrm{Td}(\overline{Tb'_g})T_g(\overline{\kappa}^{(k)})\\ &+\int_{Y_g/S}\mathrm{ch}_g(\wedge^k\overline{F}_\infty^\vee\otimes\overline{\eta}\mid_{Y_g})\mathrm{Td}^{-1}(\overline{N}_{\infty,g})\widetilde{\mathrm{Td}}(\overline{Tf_g},\overline{Tb'_g}\mid_{Y_g}).\end{aligned}$$

It is easily seen from the decomposition $\overline{\kappa}_\nabla\mid_{P_g}=\bigoplus_{k\geq 0}\overline{\kappa}_\nabla^{(k)}[-k]$ that the secondary characteristic class $\widetilde{\mathrm{ch}}_g(\overline{\kappa})$ appearing in the definition of $\delta(\overline{\kappa})$ is exactly $\sum(-1)^k\widetilde{\mathrm{ch}}_g(b'_{g_*}\overline{\kappa}^{(k)})$. So taking the alternating sum of both two sides of the equality above and using the fact that equivariant analytic torsion form is additive for direct sum of acyclic bundles, we know that to prove $\delta(\overline{\kappa})=0$, we are left to show that $\sum(-1)^kT_g(\overline{\kappa}^{(k)})$ is equal to $T_g(\overline{\kappa})$. In fact, by using [21, Lemma 3.15], we have modulo $\mathrm{Im}\partial+\mathrm{Im}\overline{\partial}$

$$\begin{aligned}\sum(-1)^kT_g(\overline{\kappa}^{(k)})&=\sum(-1)^k\mathrm{ch}_g(\wedge^k\overline{Q}_\perp^\vee)\mathrm{ch}_g(\pi_{P_g}^*\overline{\eta}\mid_{Y_g})T_g(\overline{\wedge^\cdot Q_g^\vee})\\ &=\mathrm{Td}_g^{-1}(\overline{Q}_\perp)\mathrm{ch}_g(\pi_{P_g}^*\overline{\eta}\mid_{Y_g})T_g(\overline{\wedge^\cdot Q_g^\vee})\\ &=\mathrm{Td}_g^{-1}(\overline{Q})\mathrm{ch}_g(\pi_{P_g}^*\overline{\eta}\mid_{Y_g})T_g(\overline{\wedge^\cdot Q_g^\vee})\mathrm{Td}(\overline{Q}_g)\\ &=\mathrm{ch}_g(\pi_{P_g}^*\overline{\eta}\mid_{Y_g})T_g(\overline{\wedge^\cdot Q^\vee})\\ &=T_g(\overline{\kappa}).\end{aligned}$$

So we are done. □

It's now ready to finish the proof of the vanishing theorem for equivariant closed immersions. Let $\overline{\eta}$ be an equivariant hermitian vector bundle on Y, assume that

$$\overline{\Psi}: \quad 0 \to \overline{\xi}_m \to \cdots \to \overline{\xi}_1 \to \overline{\xi}_0 \to i_*\overline{\eta} \to 0$$

is a resolution of $i_*\overline{\eta}$ by equivariant hermitian vector bundles on X which satisfies Bismut assumption (A). We need to prove that for $n \gg 0$, $\delta(\overline{\Psi}(n)) = 0$.

Proof. (of Theorem 3.1) We first construct a resolution of $p_Y^*\overline{\eta}$ on $W(i)$ as

$$\overline{\Xi}: \quad 0 \to \overline{\overline{\xi}}_m \to \cdots \to \overline{\overline{\xi}}_0 \to \overline{\overline{\xi}}_0 \to j_*p_Y^*(\overline{\eta}) \to 0$$

which satisfies the condition (i) and (ii) in Definition 3.16. Then the restriction of $\overline{\Xi}$ to X (resp. P) provides a resolution of $i_*\overline{\eta}$ (resp. $i_{\infty *}\overline{\eta}$). Over X, we can find a third resolution $\overline{\Phi}$ of $i_*\overline{\eta}$ which dominates $\overline{\Psi}$ and $\overline{\Xi}\mid_X$. Namely we get short exact sequences of exact sequences

$$0 \to \overline{\mathrm{Ker}}(n) \to \overline{\Phi}(n) \to \overline{\Psi}(n) \to 0$$

and

$$0 \to \overline{\mathrm{Ker}}'(n) \to \overline{\Phi}(n) \to \overline{\Xi}(n)\mid_X \to 0.$$

Then after omitting $i_*\overline{\eta}$ their restrictions to X_g become two exact sequences of complexes. Since $n \gg 0$ we may assume that all elements and homologies in the induced double complexes are acyclic, so that by taking direct images we get two exact sequences of equivariant standard complexes on S. These two short exact sequences of equivariant standard complexes clearly satisfy the assumptions in Lemma 3.12. Therefore, using Lemma 3.12, Bismut-Ma's immersion formula and the double complex formula of equivariant Bott-Chern singular currents (cf. Theorem 2.18), we obtain that

$$\begin{aligned}
&\widetilde{\mathrm{ch}}_g(\overline{\Psi}(n)) - \widetilde{\mathrm{ch}}_g(\overline{\Phi}(n)) + \widetilde{\mathrm{ch}}_g(\overline{\mathrm{Ker}}(n)) \\
&\qquad + T_g(\omega^{X_g}, h^{\Psi(n)_\triangledown}) - T_g(\omega^{X_g}, h^{\Phi(n)_\triangledown}) + T_g(\omega^{X_g}, h^{\mathrm{Ker}(n)_\triangledown}) \\
&= \int_{X_g/S} [T_g(\overline{\Psi}(n)_\triangledown) - T_g(\overline{\Phi}(n)_\triangledown) + T_g(\overline{\mathrm{Ker}}(n)_\triangledown)] \cdot \mathrm{Td}(\overline{Th_g})
\end{aligned}$$

which implies that

$$\delta(\overline{\Phi}(n)) = \delta(\overline{\Psi}(n)) + \delta(\overline{\mathrm{Ker}}(n)).$$

By applying Bismut-Ma's immersion formula to the case where the immersion is the identity map and $\overline{\eta}$ is equal to the zero bundle, we get $\delta(\overline{\mathrm{Ker}}(n)) = 0$ so that $\delta(\overline{\Phi}(n)) = \delta(\overline{\Psi}(n))$. Similarly, we have $\delta(\overline{\Phi}(n)) = \delta(\overline{\Xi}(n)\mid_X)$ and hence $\delta(\overline{\Psi}(n)) = \delta(\overline{\Xi}(n)\mid_X)$. An entirely analogous reasoning implies that $\delta(\overline{\kappa}(n)) = \delta(\overline{\Xi}(n)\mid_P)$. Then the vanishing of $\delta(\overline{\Psi}(n))$ follows from Theorem 3.18 and Proposition 3.19. □

4 Equivariant arithmetic Grothendieck groups with fixed wave front sets

By an arithmetic ring D we understand a regular, excellent, Noetherian integral ring, together with a finite set $\mathcal{S}$ of embeddings $D \hookrightarrow \mathbb{C}$, which is invariant under a conjugate-linear involution F_∞ (cf. [15, Def. 3.1.1]). Denote by μ_n the diagonalisable group scheme over D associated to $\mathbb{Z}/n\mathbb{Z}$. A μ_n-equivariant arithmetic scheme over D is a Noetherian scheme of finite type, endowed with a μ_n-projective action over D (cf. [21, Section 2]). Let X be a μ_n-equivariant arithmetic scheme whose generic fibre is smooth, then $X(\mathbb{C})$, the set of complex points of the variety $\coprod_{\sigma\in\mathcal{S}} X\times_D \mathbb{C}$, is a disjoint union of projective manifolds. This manifold admits an action of the group of complex n-th roots of unity and an anti-holomorphic involution induced by F_∞ which is still denoted by F_∞. It was shown in [31, Prop. 3.1] that if X is regular, then the fixed point subscheme X_{μ_n} is also regular. Fix a primitive n-th root of unity ζ_n and denote its corresponding holomorphic automorphism on $X(\mathbb{C})$ by g, by GAGA principle we have a natural isomorphism $X_{\mu_n}(\mathbb{C})\cong X(\mathbb{C})_g$.

Definition 4.1. An equivariant hermitian sheaf (resp. vector bundle) $\overline{E}$ on X is a coherent sheaf (resp. vector bundle) E on X, assumed locally free on $X(\mathbb{C})$, endowed with a μ_n-action which lifts the action of μ_n on X and a hermitian metric h on the associated bundle $E_{\mathbb{C}}$, which is invariant under F_∞ and g.

Remark 4.2. Let $\overline{E}$ be an equivariant hermitian sheaf (resp. vector bundle) on X, the restriction of $\overline{E}$ to the fixed point subscheme X_{μ_n} has a natural $\mathbb{Z}/n\mathbb{Z}$-grading structure $\overline{E}\mid_{X_{\mu_n}}\cong \oplus_{k\in\mathbb{Z}/n\mathbb{Z}}\overline{E}_k$. We shall often write $\overline{E}_{\mu_n}$ for $\overline{E}_0$. It is clear that the associated bundle of $\overline{E}_{\mu_n}$ over $X(\mathbb{C})$ is exactly equal to $\overline{E}_g$.

Over a complex manifold M, we may consider the current space which is the continuous dual of the space of smooth complex valued differential forms (cf. [27, Chapter IX]). The wave front set $\mathrm{WF}(\omega)$ of a current ω over M is a closed conical subset of the cotangent bundle $T^*_{\mathbb{R}}M_0 := T^*_{\mathbb{R}}M\backslash\{0\}$. This conical subset measures the singularities of ω, actually the projection of $\mathrm{WF}(\omega)$ in M is equal to the singular locus of the support of ω. It also allows us to define certain products and pull-backs of currents. We refer to [19, Chapter VIII] for the definition and various properties of wave front set.
Now let X be a μ_n-equivariant arithmetic scheme with smooth generic fibre and let S be a conical subset of $T^*_{\mathbb{R}}X(\mathbb{C})_{g,0}$, denote by $D^{p,p}(X(\mathbb{C})_g,S)$ the set of currents ω of type (p,p) on $X(\mathbb{C})_g$ which satisfy $F_\infty^*\omega=(-1)^p\omega$ and whose wave front sets are contained in S, we shall write $\widetilde{\mathcal{U}}(X_{\mu_n},S)$ for the current class

$$\widetilde{\mathcal{U}}(X(\mathbb{C})_g,S):=\bigoplus_{p\geq 0}(D^{p,p}(X(\mathbb{C})_g,S)/(\mathrm{Im}\partial+\mathrm{Im}\overline{\partial})).$$

Let $\overline{E}$ be an equivariant hermitian sheaf or vector bundle on X. Following the same notations and definitions as in [21, Section 3], we write $\mathrm{ch}_g(\overline{E})$ for the equivariant Chern character form $\mathrm{ch}_g((E_{\mathbb{C}},h))$ associated to the hermitian holomorphic vector bundle $(E_{\mathbb{C}},h)$ on $X(\mathbb{C})$. Similarly, we have the equivariant Todd form $\mathrm{Td}_g(\overline{E})$. Furthermore, let $\overline{\varepsilon}: 0 \to \overline{E}' \to \overline{E} \to \overline{E}'' \to 0$ be an exact sequence of equivariant hermitian sheaves or vector bundles on X, we can associate to it an equivariant Bott-Chern secondary characteristic class $\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}) \in \widetilde{\mathcal{U}}(X_{\mu_n},\emptyset)$ which satisfies the differential equation

$$\mathrm{dd}^c\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}) = \mathrm{ch}_g(\overline{E}') - \mathrm{ch}_g(\overline{E}) + \mathrm{ch}_g(\overline{E}'').$$

Definition 4.3. Let X be a μ_n-equivariant arithmetic scheme with smooth generic fibre and let S be a conical subset of $T^*_{\mathbb{R}}X(\mathbb{C})_{g,0}$, we define the equivariant arithmetic Grothendieck group $\widehat{G_0}(X,\mu_n,S)$ (resp. $\widehat{K_0}(X,\mu_n,S)$) with respect to X and S as the free abelian group generated by the elements of $\widetilde{\mathcal{U}}(X_{\mu_n},S)$ and by the equivariant isometry classes of equivariant hermitian sheaves (resp. vector bundles) on X, together with the relations
(i). for every exact sequence $\overline{\varepsilon}$ as above, $\widetilde{\mathrm{ch}}_g(\overline{\varepsilon}) = \overline{E}' - \overline{E} + \overline{E}''$;
(ii). if $\alpha \in \widetilde{\mathcal{U}}(X_{\mu_n},S)$ is the sum of two elements α' and α'' in $\widetilde{\mathcal{U}}(X_{\mu_n},S)$, then the equality $\alpha = \alpha' + \alpha''$ holds in $\widehat{G_0}(X,\mu_n,S)$ (resp. $\widehat{K_0}(X,\mu_n,S)$).

Remark 4.4. (i). When $S' \subset S$, [30, Theorem 3.9 (ii)] implies that the natural map from $\widetilde{\mathcal{U}}(X_{\mu_n},S')$ to $\widetilde{\mathcal{U}}(X_{\mu_n},S)$ is injective. So the first generating relation in Definition 4.3 does make sense.
(ii). When X is regular, one can carry out the proof of [21, Proposition 4.2] to show that the natural morphism from $\widehat{K_0}(X,\mu_n,S)$ to $\widehat{G_0}(X,\mu_n,S)$ is an isomorphism.
(iii). The definition of the equivariant arithmetic Grothendieck group implies that there are exact sequences

$$\widetilde{\mathcal{U}}(X_{\mu_n},S) \xrightarrow{a} \widehat{G_0}(X,\mu_n,S) \xrightarrow{\pi} G_0(X,\mu_n) \longrightarrow 0$$

and

$$\widetilde{\mathcal{U}}(X_{\mu_n},S) \xrightarrow{a} \widehat{K_0}(X,\mu_n,S) \xrightarrow{\pi} K_0(X,\mu_n) \longrightarrow 0$$

where a is the natural map which sends $\alpha \in \widetilde{\mathcal{U}}(X_{\mu_n},S)$ to the class of α in $\widehat{G_0}(X,\mu_n,S)$ (resp. $\widehat{K_0}(X,\mu_n,S)$) and π is the forgetful map. Here the group $G_0(X,\mu_n)$ is the Grothendieck group of μ_n-equivariant coherent sheaves which are locally free on $X(\mathbb{C})$, by a theorem of Quillen (cf. [26, Thm. 3 Cor. 1]) we know that it is isomorphic to the ordinary Grothendieck group of μ_n-equivariant coherent sheaves.

In [29, Section 3], we have introduced the ring structure of $\widehat{K_0}(X,\mu_n,\emptyset)$. Since we may have a well-defined product of two currents if their wave front sets have no intersection, and the wave front set is invariant under the operation of multiplying a smooth current, we know that the Grothendieck group $\widehat{K_0}(X,\mu_n,S)$ has a $\widehat{K_0}(X,\mu_n,\emptyset)$-module structure. The same thing goes to $\widehat{G_0}(X,\mu_n,S)$.

Furthermore, consider the isomorphism $R(\mu_n) \cong K_0(D)[T]/(1-T^n)$. Let $\overline{I}$ be the μ_n-equivariant hermitian D-module whose term of degree 1 is D endowed with the trivial metric and whose other terms are 0. Then we may make $\widehat{K_0}(D,\mu_n,\emptyset)$ an $R(\mu_n)$-algebra under the ring morphism which sends T to $\overline{I}$. By doing pull-backs, we may endow every arithmetic Grothendieck group we defined before with an $R(\mu_n)$-module structure. Notice finally that there is a well-defined map from $\widehat{G_0}(X,\mu_n,\emptyset)$ (resp. $\widehat{K_0}(X,\mu_n,\emptyset)$) to the space of complex closed differential forms, which is defined by the formula $\mathrm{ch}_g(\overline{E}+\alpha) := \mathrm{ch}_g(\overline{E}) + \mathrm{dd}^c\alpha$ where $\overline{E}$ is an equivariant hermitian sheaf (resp. vector bundle) and $\alpha \in \widetilde{\mathcal{U}}(X_{\mu_n},\emptyset)$.

Now we investigate the wave front set of a current after doing push-forward. Let f be a holomorphic map of compact complex manifolds, we may define a push-forward f_* on current space which is the dual map of the pull-back of smooth forms. When f is smooth, the push-forward f_* extends the integration of smooth forms over the fibre. Assume that we are given a smooth morphism $f: U \to V$ of compact complex manifolds, then f_* induces a current K over the product space $V \times U$ defined as

$$K(\alpha \otimes \beta) = (f_*\beta)(\alpha)$$

where α and β are smooth forms over V and U respectively. Define

$$M = \{(v,u) \in V \times U \mid f(u) = v\}$$

which is a submanifold in $V \times U$. From the fact that $f_*\beta$ is just the integration of smooth forms over the fibre, it is easily seen that the current $K \in D^*(V \times U)$ is exactly the object $\mathrm{d}S_M$ in [19, Theorem 8.1.5]. Then by that theorem, the wave front set of K is equal to

$$\mathrm{WF}(K) = \{(v,u,\xi,-f^*(\xi)) \in T^*_{\mathbb{R}}V \times T^*_{\mathbb{R}}U \mid f(u) = v, \xi \neq 0\}.$$

Let S be a conical subset of $T^*_{\mathbb{R}}U_0$, we fix some notations as follows.

$$\begin{aligned}
\mathrm{WF}(K)_V =& \{(v,\xi) \in T^*_{\mathbb{R}}V_0 \mid \exists u \in U, (v,u,\xi,0) \in \mathrm{WF}(K)\}\\
\mathrm{WF}'(K)_U =& \{(u,\eta) \in T^*_{\mathbb{R}}U_0 \mid \exists v \in V, (v,u,0,-\eta) \in \mathrm{WF}(K)\}\\
\mathrm{WF}'(K)_V \circ S =& \{(v,\xi) \in T^*_{\mathbb{R}}V_0 \mid \exists (u,\eta) \in S, (v,u,\xi,-\eta) \in \mathrm{WF}(K)\}.
\end{aligned}$$

Theorem 4.5. *Let notations and assumptions be as above. Assume that ω is a current over U whose wave front set is contained in S with $S \cap \mathrm{WF}'(K)_U = \emptyset$, then the wave front set of $f_*\omega$ is contained in*

$$S' := \mathrm{WF}(K)_V \cup \mathrm{WF}'(K) \circ S.$$

Proof. This follows from [19, Theorem 8.2.12 and 8.2.13]. □

Remark 4.6. (i) In our situation, the condition $S \cap \mathrm{WF}'(K)_U = \emptyset$ is always satisfied because by definition we have $\mathrm{WF}'(K)_U = \emptyset$.

(ii). In our situation, S' is always equal to $\mathrm{WF}'(K)\circ S$ because $\mathrm{WF}(K)_V=\emptyset$.
(iii). If S is the empty set, then S' is also empty. This is compatible with the push-forward of smooth forms.
(iv). Assume that the restriction of f to a closed submanifold W is also smooth. Denote by $N_{U/W}$ the normal bundle of W in U. If $S=N_{U/W,\mathbb{R}}^\vee\setminus\{0\}$, then $S'=\emptyset$.

We now turn to the arithmetic case. Let X,Y be two μ_n-equivariant arithmetic schemes with smooth generic fibres, and let $f:X\to Y$ be an equivariant morphism over D which is smooth on the complex numbers. Fix a $\mu_n(\mathbb{C})$-invariant Kähler metric on $X(\mathbb{C})$ so that we get a Kähler fibration with respect to the holomorphic submersion $f_{\mathbb{C}}:X(\mathbb{C})\to Y(\mathbb{C})$. Let $\overline{E}$ be an f-acyclic μ_n-equivariant hermitian sheaf on X, we know that the direct image f_*E is locally free on $Y(\mathbb{C})$ and it can be endowed with a natural equivariant structure and the L^2-metric. Let $\widehat{G_0}^{\mathrm{ac}}(X,\mu_n,S)$ be the group generated by f-acyclic equivariant hermitian sheaves on X and the elements of $\widetilde{\mathcal{U}}(X_{\mu_n},S)$, with the same relations as in Definition 4.3. A theorem of Quillen (cf. [26, Cor.3 P. 111]) for the algebraic analogs of these groups implies that the natural map $\widehat{G_0}^{\mathrm{ac}}(X,\mu_n,S)\to\widehat{G_0}(X,\mu_n,S)$ is an isomorphism. So the following definition does make sense.

Definition 4.7. Let notations and assumptions be as above. The push-forward morphism $f_*:\widehat{G_0}(X,\mu_n,S)\to\widehat{G_0}(Y,\mu_n,S')$ is defined in the following way.
(i). For every f-acyclic μ_n-equivariant hermitian sheaf $\overline{E}$ on X, $f_*\overline{E}=(f_*E,f_*h^E)-T_g(\omega^X,h^E)$.
(ii). For every element $\alpha\in\widetilde{\mathcal{U}}(X_{\mu_n},S)$, $f_*\alpha=\int_{X_g/Y_g}\mathrm{Td}_g(Tf,h^{Tf})\alpha\in\widetilde{\mathcal{U}}(Y_{\mu_n},S')$.

Remark 4.8. If Y is regular, by Remark 4.4 (ii) we know that $\widehat{K_0}(Y,\mu_n,S')$ is naturally isomorphic to $\widehat{G_0}(Y,\mu_n,S')$ so that (f_*E,f_*h^E) admits a finite equivariant hermitian resolution; if the morphism f is flat and Y is reduced, then (f_*E,f_*h^E) is locally free when E is so. Therefore in both two cases above, one can also define a reasonable push-forward morphism $f_*:\widehat{K_0}(X,\mu_n,S)\to\widehat{K_0}(Y,\mu_n,S')$.

Theorem 4.9. *The push-forward morphism f_* is a well-defined group homomorphism.*

Proof. The argument is the same as in the proof of [29, Theorem 6.2]. □

Lemma 4.10. *(Projection formula) For any elements $y\in\widehat{K_0}(Y,\mu_n,\emptyset)$ and $x\in\widehat{G_0}(X,\mu_n,S)$, the identity $f_*(f^*y\cdot x)=y\cdot f_*x$ holds in $\widehat{G_0}(Y,\mu_n,S')$.*

Proof. Assume that $y=\overline{E}$ is an equivariant hermitian vector bundle and $x=\overline{F}$ is an f-acyclic equivariant hermitian sheaf, then $f^*y\cdot x=f^*\overline{E}\otimes\overline{F}$. By projection formula for direct images and the definition of L^2-metric, we know that $f_*(f^*\overline{E}\otimes\overline{F})$ is isometric to $\overline{E}\otimes f_*\overline{F}$. Moreover, concerning the analytic torsion form, we have $T_g(\omega^X, h^{f^*E\otimes F}) = \mathrm{ch}_g(\overline{E})T_g(\omega^X, h^F)$. So the projection formula $f_*(f^*y\cdot x) = y\cdot f_*x$ holds in this case.

Assume that $y = \overline{E}$ is an equivariant hermitian vector bundle and $x = \alpha$ is represented by some singular current. We write f_g^* and f_{g*} for the pull-back and push-forward of currents respectively, then

$$\begin{aligned} f_*(f^*y\cdot x) =& f_*(f_g^*\mathrm{ch}_g(\overline{E})\alpha) = f_{g*}(f_g^*\mathrm{ch}_g(\overline{E})\alpha\mathrm{Td}_g(\overline{Tf}))\\ =&\mathrm{ch}_g(\overline{E})f_{g*}(\alpha\mathrm{Td}_g(\overline{Tf}))\\ =&\mathrm{ch}_g(\overline{E})\int_{X_g/Y_g}\alpha\mathrm{Td}_g(\overline{Tf}) = y\cdot f_*x.\end{aligned}$$

Here we have used an extension of projection formula of smooth forms $p_*(p^*\alpha_1\wedge\alpha_2) = \alpha_1\wedge p_*\alpha_2$ (cf. [14, Prop. IX p. 303]) to the case where the second variable α_2 is replaced by a singular current. The fact that this extension is valid follows from the definition of p_* and the definition of the product of smooth form and singular current.

Assume that $y = \beta$ is represented by some smooth form and $x = \overline{E}$ is an f-acyclic hermitian sheaf, then

$$\begin{aligned} f_*(f^*y\cdot x) =& f_*(f_g^*(\beta)\mathrm{ch}_g(\overline{F})) = f_{g*}(f_g^*(\beta)\mathrm{ch}_g(\overline{F})\mathrm{Td}_g(\overline{Tf}))\\ =&\beta f_{g*}(\mathrm{ch}_g(\overline{E})\mathrm{Td}_g(\overline{Tf}))\\ =&\beta\int_{X_g/Y_g}\mathrm{ch}_g(\overline{E})\mathrm{Td}_g(\overline{Tf}) = \beta(\mathrm{ch}_g(\overline{f_*F}) - \mathrm{dd}^cT_g(\omega^X, h^F))\end{aligned}$$

which is exactly $y\cdot f_*x$.

Finally, assume that $y = \beta$ is represented by some smooth form and $x = \alpha$ is represented by some singular current, then

$$\begin{aligned} f_*(f^*y\cdot x) =& f_*(f_g^*(\beta)\mathrm{dd}^c\alpha) = f_{g*}(f_g^*(\beta)\mathrm{dd}^c\alpha\mathrm{Td}_g(\overline{Tf}))\\ =&\beta\mathrm{dd}^c f_{g*}(\alpha\mathrm{Td}_g(\overline{Tf}))\end{aligned}$$

which is also equal to $y\cdot f_*x$.

Since f_* and f^* are both group homomorphisms, we may conclude the projection formula by linear extension. □

REMARK 4.11. Lemma 4.10 implies that f_* is a homomorphism of $R(\mu_n)$-modules, and hence it induces a push-forward morphism after taking localization.

To end this section, we recall an important lemma which will be used frequently in our later arguments.

LEMMA 4.12. *([21, Lemma 4.5]) Let X be a regular μ_n-equivariant arithmetic scheme and let $\overline{E}$ be an equivariant hermitian vector bundle on X_{μ_n} such that $\overline{E}_{\mu_n} = 0$. Then the element $\lambda_{-1}(\overline{E})$ is invertible in $\widehat{K_0}(X_{\mu_n}, \mu_n, S)_\rho$.*

5 Arithmetic concentration theorem

In this section, we shall prove the arithmetic concentration theorem which is an analog of Thomason's result in Arakelov geometry. Let X be a μ_n-equivariant arithmetic scheme with smooth generic fibre, we consider a special closed immersion $i : X_{\mu_n} \hookrightarrow X$ where X_{μ_n} is the fixed point subscheme of X. We shall first construct a well-defined group homomorphism i_* between equivariant arithmetic G_0-groups as in the algebraic case. To construct i_*, some analytic datum, which is the equivariant Bott-Chern singular current, should be involved. Precisely speaking, let $\overline{\eta}$ be a μ_n-equivariant hermitian sheaf on X_{μ_n} and let $\overline{\xi}.$ be a bounded complex of μ_n-equivariant hermitian sheaves which provides a resolution of $i_*\overline{\eta}$ on X. Such a resolution always exists since the generic fibre of X is supposed to be smooth. Then we may have an equivariant Bott-Chern singular current $T_g(\overline{\xi}.) \in \widetilde{\mathcal{U}}(X_{\mu_n})$. Note that on the complex numbers the 0-degree part of the normal bundle $N := N_{X/X_g}$ vanishes (cf. [21, Prop. 2.12]) so that the wave front set of $T_g(\overline{\xi}.)$ is the empty set. This fact means that the following definition does make sense.

Definition 5.1. Let notations and assumptions be as above. The embedding morphism

$$i_* : \quad \widehat{G_0}(X_{\mu_n}, \mu_n, S) \to \widehat{G_0}(X, \mu_n, S)$$

is defined in the following way.
(i). For every μ_n-equivariant hermitian sheaf $\overline{\eta}$ on X_{μ_n}, suppose that $\overline{\xi}.$ is a resolution of $i_*\overline{\eta}$ on X whose metrics satisfy Bismut assumption (A), $i_*[\overline{\eta}] = \sum_k (-1)^k[\overline{\xi}_k] + T_g(\overline{\xi}.)$.
(ii). For every $\alpha \in \widetilde{\mathcal{U}}(X_{\mu_n}, S)$, $i_*\alpha = \alpha \mathrm{Td}_g^{-1}(\overline{N})$.

Theorem 5.2. *The embedding morphism i_* is a well-defined group homomorphism.*

Proof. The argument is the same as in the proof of [29, Theorem 5.2]. □

Lemma 5.3. *(Projection formula) For any elements $x \in \widehat{K_0}(X, \mu_n, \emptyset)$ and $y \in \widehat{G_0}(X_{\mu_n}, \mu_n, S)$, the identity $i_*(i^*x \cdot y) = x \cdot i_*y$ holds in $\widehat{G_0}(X, \mu_n, S)$.*

Proof. Assume that $x = \overline{E}$ is an equivariant hermitian vector bundle and $y = \overline{F}$ is an equivariant hermitian sheaf. Let $\overline{\xi}.$ be a resolution of $i_*\overline{F}$ on X, then $\overline{E} \otimes \overline{\xi}.$ provides a resolution of $i_*(i^*\overline{E} \otimes \overline{F})$. By definition we have

$$i_*(i^*x \cdot y) = \sum (-1)^k[\overline{\xi}_k \otimes \overline{E}] + \mathrm{ch}_g(\overline{E}) T_g(\overline{\xi}.)$$

which is exactly $x \cdot i_*y$. Assume that $x = \alpha$ is represented by some smooth form and $y = \overline{F}$ is an equivariant hermitian sheaf. Again let $\overline{\xi}.$ be a resolution of $i_*\overline{F}$ on X, then

$$i_*(i^*x \cdot y) = \alpha \mathrm{Td}_g^{-1}(\overline{N}_{X/X_g}) \mathrm{ch}_g(\overline{F}) = \alpha[\mathrm{dd}^c T_g(\overline{\xi}.) + \sum (-1)^k \mathrm{ch}_g(\overline{\xi}_k)]$$

which is exactly $x \cdot i_* y$. Now assume that $x = \overline{E}$ is an equivariant hermitian vector bundle and $y = \alpha$ is represented by some singular current, then

$$i_*(i^* x \cdot y) = i_*(\mathrm{ch}_g(\overline{E})\alpha) = \mathrm{ch}_g(\overline{E})\alpha \mathrm{Td}_g^{-1}(\overline{N}_{X/X_g})$$

which is exactly $x \cdot i_* y$. Finally, if x is represented by some smooth form and y is represented by some singular current then their product is well-defined and $i_*(i^* x \cdot y)$ is obviously equal to $x \cdot i_* y$. Note that i_* and i^* are group homomorphisms, so we may conclude the projection formula from its correctness on generators. This completes the proof. □

Remark 5.4. Lemma 5.3 implies that i_* is even a homomorphism of $R(\mu_n)$-modules so that it induces a homomorphism between arithmetic G_0-groups after taking localization.

With Remark 5.4, we may formulate the arithmetic concentration theorem as follows.

Theorem 5.5. *The embedding morphism* $i_* : \widehat{K_0}(X_{\mu_n}, \mu_n, S)_\rho \to \widehat{K_0}(X, \mu_n, S)_\rho$ *is an isomorphism if* X *is regular. In this case, the inverse morphism of* i_* *is given by* $\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_{\mu_n}}) \cdot i^*$ *where* $N_{X/X_{\mu_n}}$ *is the normal bundle of* $i(X_{\mu_n})$ *in* X.

Before we give the proof of this concentration theorem, we recall a crucial lemma as follows.

Lemma 5.6. *Let* $\overline{\eta}$ *be an equivariant hermitian vector bundle on* X_{μ_n}. *Assume that* $\overline{\xi.}$ *is an equivariant hermitian resolution of* $i_*\overline{\eta}$ *on* X *whose metrics satisfy Bismut assumption (A). Then the equality*

$$\lambda_{-1}(\overline{N}^\vee_{X/X_{\mu_n}}) \cdot \overline{\eta} - \sum_j (-1)^j i^*(\overline{\xi}_j) = T_g(\overline{\xi}.)$$

holds in the group $\widehat{K_0}(X_{\mu_n}, \mu_n, S)$.

Proof. This is [29, Lemma 5.13]. □

Proof. (of Theorem 5.5) Denote by U the complement of X_{μ_n} in X, then $j : U \hookrightarrow X$ is a μ_n-equivariant open subscheme of X whose fixed point set is empty. We consider the following double complex

$$\begin{array}{ccccccc}
\widetilde{\mathcal{U}}(X_{\mu_n},S)_\rho & \xrightarrow{i_*} & \widetilde{\mathcal{U}}(X_{\mu_n},S)_\rho & \xrightarrow{j^*} & \widetilde{\mathcal{U}}(U_{\mu_n},\emptyset)_\rho & \longrightarrow & 0 \\
\downarrow{\scriptstyle a} & & \downarrow{\scriptstyle a} & & \downarrow{\scriptstyle a} & & \\
\widehat{K_0}(X_{\mu_n},\mu_n,S)_\rho & \xrightarrow{i_*} & \widehat{K_0}(X,\mu_n,S)_\rho & \xrightarrow{j^*} & \widehat{K_0}(U,\mu_n,\emptyset)_\rho & \longrightarrow & 0 \\
\downarrow{\scriptstyle \pi} & & \downarrow{\scriptstyle \pi} & & \downarrow{\scriptstyle \pi} & & \\
K_0(X_{\mu_n},\mu_n)_\rho & \xrightarrow{i_*} & K_0(X,\mu_n)_\rho & \xrightarrow{j^*} & K_0(U,\mu_n)_\rho & \longrightarrow & 0 \\
\downarrow & & \downarrow & & \downarrow & & \\
0 & & 0 & & 0 & &
\end{array}$$

whose first and second columns are both exact sequences according to Remark 4.4 (iii). For the third column, $K_0(U,\mu_n)_\rho$ is equal to 0 by [31, (2.1.3)], $\widetilde{\mathcal{U}}(U_{\mu_n},\emptyset)_\rho$ is also equal to 0 since U_{μ_n} is empty. Then from Remark 4.4 (iii) we know that $\widehat{K_0}(U,\mu_n,\emptyset)_\rho$ is equal to 0. We claim that $i_*:\widehat{K_0}(X_{\mu_n},\mu_n,S)_\rho\to\widehat{K_0}(X,\mu_n,S)_\rho$ is surjective. Indeed, for any element $x\in\widehat{K_0}(X,\mu_n,S)_\rho$ we may find an element $y\in\widehat{K_0}(X_{\mu_n},\mu_n,S)_\rho$ such that $i_*\pi(y)=\pi(x)$ because the third line is exact. This means $x-i_*(y)$ is in the kernel of π, so there exists an element $\alpha\in\widetilde{\mathcal{U}}(X_{\mu_n},S)_\rho$ such that $\alpha=x-i_*(y)$ in $\widehat{K_0}(X,\mu_n,S)_\rho$. Set $\beta=\alpha\mathrm{Td}_g(\overline{N})$, we get $i_*(y+\beta)=i_*(y)+\alpha=x$ in $\widehat{K_0}(X,\mu_n,S)_\rho$. Hence, i_* is surjective.

We now prove that the embedding morphism $i_*:\widehat{K_0}(X_{\mu_n},\mu_n,S)_\rho\to\widehat{K_0}(X,\mu_n,S)_\rho$ is really an isomorphism by constructing its inverse morphism. Let ω be an element in $\widetilde{\mathcal{U}}(X_{\mu_n},S)$, by definition we have

$$\begin{aligned}\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_{\mu_n}})\cdot i^*i_*(\omega)=&\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_{\mu_n}})\cdot\omega\mathrm{Td}_g^{-1}(\overline{N}_{X/X_g})\\ =&\mathrm{ch}_g(\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_g}))\omega\mathrm{Td}_g^{-1}(\overline{N}_{X/X_g})\\ =&\omega.\end{aligned}$$

Let $\overline{\eta}$ be an equivariant hermitian vector bundle on X_{μ_n} and assume that $\overline{\xi.}$ is an equivariant hermitian resolution of $i_*\overline{\eta}$ on X whose metrics satisfy Bismut assumption (A), then by the definition of the embedding morphism i_* and Lemma 5.6 we have

$$\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_{\mu_n}})\cdot i^*i_*(\overline{\eta})=\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_{\mu_n}})\cdot i^*(\sum_k(-1)^k\overline{\xi}_k+T_g(\overline{\xi.}))=\overline{\eta}.$$

So the inverse morphism of i_* is of the form $\lambda_{-1}^{-1}(\overline{N}^\vee_{X/X_{\mu_n}})\cdot i^*$ and we are done. □

6 A Lefschetz fixed point formula for singular arithmetic schemes with smooth generic fibres

6.1 The statement

We formulate in this subsection the statement of our main theorem, a singular Lefschetz fixed point formula for equivariant arithmetic schemes with smooth generic fibres. Its proof will be given in next two subsections. Let $f : X \to Y$ be a μ_n-equivariant morphism between two arithmetic schemes with smooth generic fibres, which is smooth on the complex numbers. This morphism f is automatically projective and hence proper, according to the definition of equivariant arithmetic scheme. Suppose that f factors through some regular equivariant arithmetic scheme Z. More precisely, our assumption is that there exist an equivariant closed immersion $i : X \hookrightarrow Z$ and an equivariant morphism $h : Z \to Y$ such that $f = h \circ i$ and h is also smooth on the complex numbers. Moreover, we shall assume that the μ_n-action on Y is trivial.
Let η be an equivariant coherent sheaf on X, then there exists a bounded complex of equivariant vector bundles which provides a resolution of $i_*\eta$ on Z because Z is regular. Since any two equivariant resolution of $i_*\eta$ can be dominated by a third one, the symbol $\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\eta, \mathcal{O}_{Z_{\mu_n}})$ does make sense.
We choose arbitrary μ_n-invariant Kähler forms ω^Z and ω^X on $Z(\mathbb{C})$ and $X(\mathbb{C})$ respectively, the Kähler form ω^X is not necessarily the Kähler form induced by ω^Z. The Kähler form on $X(\mathbb{C})$ induced by ω^Z will be denoted by ω^Z_X. Denote by N the normal bundle of $i_{\mathbb{C}}(X(\mathbb{C}))$ in $Z(\mathbb{C})$, we endow it with the quotient metric provided that $TX(\mathbb{C})$ carries the Kähler metric corresponding to ω^Z_X. Let $\overline{F}$ be the non-zero degree part of $\overline{N}$, then by [13, Exp. VII, Lem. 2.4 and Prop. 2.5] for any equivariant hermitian sheaf $\overline{\eta}$ on X there exists a canonical isomorphism on X_g

$$\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\eta, \mathcal{O}_{Z_{\mu_n}})_{\mathbb{C}} \cong \wedge^k F^\vee \otimes \eta_{\mathbb{C}} \mid_{X_g}$$

which is equivariant. This means we may endow $\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\eta, \mathcal{O}_{Z_{\mu_n}})_{\mathbb{C}}$ with a hermitian metric induced by the metrics on F and η so that it becomes an equivariant hermitian sheaf on X_{μ_n}. Moreover, we know that the hermitian vector bundle $\overline{F}$ fits the following exact sequence

$$(\overline{\mathcal{F}}, \omega^X): \quad 0 \to \overline{N}_{X/X_g} \to \overline{N}_{Z/Z_g} \to \overline{F} \to 0$$

where N_{Z/Z_g} admits the quotient metric associated to ω^Z and N_{X/X_g} admits the quotient metric associated to ω^X. Similarly, we shall denote by $(\overline{\mathcal{F}}, \omega^Z_X)$ the hermitian exact sequence $\overline{\mathcal{F}}$ whose metric on N_{X/X_g} is induced by ω^Z_X.
The push-forward homomorphism from the arithmetic G_0-group $\widehat{G_0}(X, \mu_n, \emptyset)$ to $\widehat{G_0}(Y, \mu_n, \emptyset)$ with respect to the Kähler form ω^X is denoted by f_* as usual. The push-forward homomorphism from $\widehat{G_0}(X_{\mu_n}, \mu_n, \emptyset)$ to $\widehat{G_0}(Y, \mu_n, \emptyset)$ with respect to the Kähler form ω^Z_X will be denoted by $f^Z_{\mu_n *}$.

Write $\widetilde{\mathrm{Td}}(Tf_g,\omega^X,\omega_X^Z)$ for the secondary characteristic class of the exact sequence

$$0 \longrightarrow (Tf_g,\omega^X) \xrightarrow{\mathrm{Id}} (Tf_g,\omega_X^Z) \longrightarrow 0 \longrightarrow 0$$

where the middle term carries the metric induced by ω_X^Z and the sub term carries the metric induced by ω^X. Then the singular Lefschetz fixed point formula for equivariant arithmetic schemes with smooth generic fibres can be formulated as follows.

Theorem 6.1. *Let notations and assumptions be as above. Then for any equivariant hermitian sheaf $\overline{\eta}$ on X, the equality*

$$\begin{aligned} f_*(\overline{\eta}) =& f^Z_{\mu_n *}(i^*_{\mu_n}(\lambda_{-1}^{-1}(\overline{N}^\vee_{Z/Z_{\mu_n}}))\cdot\sum_k(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}})) \\ &+\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^X)\mathrm{Td}_g^{-1}(\overline{F}) \\ &-\int_{X_g/Y}\mathrm{Td}_g(Tf)\mathrm{ch}_g(\eta)R_g(N_{X/X_g}) \\ &+\int_{X_g/Y}\widetilde{\mathrm{Td}}(Tf_g,\omega^X,\omega_X^Z)\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\mathrm{Td}_g^{-1}(\overline{F}) \end{aligned}$$

holds in the group $\widehat{G_0}(Y,\mu_n,\emptyset)_\rho$.

Remark 6.2. This arithmetic Lefschetz fixed point formula was inspired by [31, Théorème 3.5].

6.2 Equivariant arithmetic G_0-theoretic vanishing theorem

The central actor in the proof of Theorem 6.1 is the following vanishing theorem in equivariant arithmetic G_0-theory, which can be viewed as a translation of Theorem 3.1.

Theorem 6.3. *Let notations and assumptions be as in last subsection. Let $\overline{\eta}$ be an equivariant hermitian sheaf on X, and let*

$$\overline{\Psi}:\quad 0\to\overline{\xi}_m\to\cdots\to\overline{\xi}_1\to\overline{\xi}_0\to i_*\overline{\eta}\to 0$$

be a resolution of $i_*\overline{\eta}$ by equivariant hermitian vector bundles on Z. Denote by $h_{\mu_n *}$ the push-forward homomorphism from $\widehat{K_0}(Z_{\mu_n},\mu_n,N^\vee_{g,\mathbb{R}}\setminus\{0\})$ to $\widehat{G_0}(Y,\mu_n,\emptyset)$ with respect to the Kähler form ω^Z. Then the formula

$$\begin{aligned} & f^Z_{\mu_n *}(\sum(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}}))-h_{\mu_n *}(\sum(-1)^k(\overline{\xi}_k\mid_{Z_{\mu_n}})) \\ =& \int_{Z_g/Y}T_g(\overline{\xi}.)\mathrm{Td}(\overline{Th_g})+\int_{X_g/Y}\mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g) \\ &+\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g}) \end{aligned}$$

holds in $\widehat{G_0}(Y, \mu_n, \emptyset)$.

Proof. Following the same arguments given in the proof of Lemma 3.9, we may show that the deformation to the normal cone $W(i)$ admits an equivariant hermitian very ample invertible sheaf $\overline{\mathcal{L}}$ which is relative to the morphism $l : W(i) \to Y$. By Theorem 3.1 and the fact that $\mathcal{L}$ is very ample, we conclude that there exists an integer $k_0 > 0$ such that for $n \geq k_0$, $\mathcal{L}^{\otimes n}$ is l-acyclic and $\delta(\overline{\Psi}(n)_{\mathbb{C}}) = 0$. Then l factors through an equivariant projective space bundle $\mathbb{P}(\mathcal{E})$ where $\mathcal{E}$ is locally free of rank $r+1$ on Y and $l_*\mathcal{L}^{\otimes k_0}$ is an equivariant quotient of $\mathcal{E}$. Denote by $p : \mathbb{P}(\mathcal{E}) \to Y$ the canonical projection. On $P := \mathbb{P}(\mathcal{E})$, we have a canonical exact sequence

$$\mathcal{H}: \quad 0 \to \mathcal{O}_P \to p^*(\mathcal{E}^\vee)(1) \to \cdots \to p^*(\wedge^{r+1}\mathcal{E}^\vee)(r+1) \to 0.$$

Restricting this sequence to Z, we obtain an exact sequence of exact sequences

$$0 \to \Psi \to \Psi \otimes h^*(\mathcal{E}^\vee)(1) \to \cdots \to \Psi \otimes h^*(\wedge^{r+1}\mathcal{E}^\vee)(r+1) \to 0.$$

Endow $\mathcal{E}$ with any $\mu_n(\mathbb{C})$-invariant hermitian metric. We claim that the assumption that Theorem 6.3 holds for $\overline{\Psi} \otimes h^*(\wedge^n \overline{\mathcal{E}}^\vee)(n)$ with $n \geq 1$ implies that it holds for $\overline{\Psi}$. In fact, since $\mathcal{H}$ is an exact sequence of flat modules, for any $k \geq 0$ we have the following exact sequence on X_{μ_n}

$$\begin{aligned} 0 \to \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}}) \to & \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}}) \otimes f^*_{\mu_n}(\overline{\mathcal{E}}^\vee)(1) \to \cdots \\ \to & \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}}) \otimes f^*_{\mu_n}(\wedge^{r+1}\overline{\mathcal{E}}^\vee)(r+1) \to 0. \end{aligned}$$

We compute

$$\begin{aligned} & f^Z_{\mu_n *}(\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}})) \\ = & f^Z_{\mu_n *}(-\sum_{j=1}^{r+1}(-1)^j \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}}) \otimes f^*_{\mu_n}(\wedge^j \overline{\mathcal{E}}^\vee)(j)) \\ & + \int_{X_g/Y} \mathrm{Td}(Tf_g, \omega^Z_X)\mathrm{ch}_g(\wedge^k \overline{F}^\vee)\mathrm{ch}_g(\overline{\eta})(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}}) \end{aligned}$$

and

$$\begin{aligned} & \sum_{k=0}^m (-1)^k h_{\mu_n *}(\overline{\xi}_k \mid_{Z_{\mu_n}}) \\ = & \sum_{k=0}^m (-1)^k h_{\mu_n *}(-\sum_{j=1}^{r+1}(-1)^j \overline{\xi}_k \mid_{Z_{\mu_n}} \otimes h^*_{\mu_n}(\wedge^j \overline{\mathcal{E}}^\vee)(j)) \\ & + \sum_{k=0}^m (-1)^k \int_{Z_g/Y} \mathrm{Td}(\overline{Th_g})\mathrm{ch}_g(\overline{\xi}_k)(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}}). \end{aligned}$$

Moreover, we have

$$\int_{X_g/Y}\mathrm{Td}(Tf_g)\mathrm{ch}_g(\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\eta,\mathcal{O}_{Z_{\mu_n}}))R(N_g)$$
$$=\int_{X_g/Y}-\sum_{j=1}^{r+1}(-1)^j\mathrm{ch}_g(\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\eta,\mathcal{O}_{Z_{\mu_n}})\otimes f^*_{\mu_n}(\wedge^j\mathcal{E}^\vee)(j))R(N_g)\mathrm{Td}(Tf_g)$$

and

$$\int_{Z_g/Y}T_g(\overline{\xi}.)\mathrm{Td}(\overline{Th_g})$$
$$=\int_{Z_g/Y}\mathrm{Td}(\overline{Th_g})\{\delta_{X_g}\mathrm{Td}_g^{-1}(\overline{N})\mathrm{ch}_g(\overline{\eta})(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})$$
$$-\sum_{k=0}^{m}(-1)^k\mathrm{ch}_g(\overline{\xi}_k)(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})-\sum_{j=1}^{r+1}(-1)^jT_g(\overline{\xi}.)\mathrm{ch}_g(h^*_{\mu_n}(\wedge^j\overline{\mathcal{E}}^\vee)(j))\}$$

by the double complex formula of equivariant Bott-Chern singular currents. At last, we also have

$$\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g})$$
$$=\int_{X_g/Y}\{\mathrm{dd}^c(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})\mathrm{ch}_g(\overline{\eta})-\sum_{j=1}^{r+1}(-1)^j\mathrm{ch}_g(\overline{\eta}\otimes f^*(\wedge^j\overline{\mathcal{E}}^\vee)(j))\}$$
$$\cdot\,\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g})$$
$$=-\int_{X_g/Y}(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})\mathrm{ch}_g(\overline{\eta})\cdot\{\mathrm{Td}_g^{-1}(\overline{N})\mathrm{Td}(\overline{Th_g})$$
$$-\mathrm{Td}(Tf_g,\omega_X^Z)\mathrm{Td}_g^{-1}(\overline{F})\}$$
$$-\int_{X_g/Y}\sum_{j=1}^{r+1}(-1)^j\mathrm{ch}_g(\overline{\eta}\otimes f^*(\wedge^j\overline{\mathcal{E}}^\vee)(j))\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g}).$$

Gathering all these computations above and using our assumption, we get

$$f^Z_{\mu_n *}(\sum(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}}))-h_{\mu_n *}(\sum(-1)^k\overline{\xi}_k\mid_{Z_{\mu_n}})$$
$$-\int_{Z_g/Y}T_g(\overline{\xi}.)\mathrm{Td}(\overline{Th_g})-\int_{X_g/Y}\mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)$$
$$-\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g})$$
$$=\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega_X^Z)\mathrm{Td}_g^{-1}(\overline{F})\mathrm{ch}_g(\overline{\eta})(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})$$

$$- \sum_{k=0}^{m}(-1)^k \int_{Z_g/Y} \mathrm{Td}(\overline{Th_g})\mathrm{ch}_g(\overline{\xi}_k)(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})$$
$$- \int_{X_g/Y} \mathrm{Td}(\overline{Th_g})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{ch}_g(\overline{\eta})(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})$$
$$+ \sum_{k=0}^{m}(-1)^k \int_{Z_g/Y} \mathrm{Td}(\overline{Th_g})\mathrm{ch}_g(\overline{\xi}_k)(-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})$$
$$+ \int_{X_g/Y} (-1)^{r+1}\widetilde{\mathrm{ch}}_g(\overline{\mathcal{H}})\mathrm{ch}_g(\overline{\eta})\{\mathrm{Td}_g^{-1}(\overline{N})\mathrm{Td}(\overline{Th_g}) - \mathrm{Td}(Tf_g,\omega_X^Z)\mathrm{Td}_g^{-1}(\overline{F})\}$$

which vanishes. This ends the proof of our claim.
By the construction of the projective space bundle P, we have already known that $\delta(\overline{\Psi}(n)_{\mathbb{C}})$ vanishes from $n = 1$ to $n = r + 1$. Moreover, according to the projection formula of higher direct images, the operation of tensoring with the element $l^*(\wedge^n\overline{\mathcal{E}}^\vee)$ doesn't change the property of l-acyclicity. Hence we also have $\delta(\overline{\Psi} \otimes h^*(\wedge^n\overline{\mathcal{E}}^\vee)(n)_{\mathbb{C}}) = 0$. By the generating relations and the definition of push-forward morphisms of arithmetic G_0-groups, this is equivalent to say that Theorem 6.3 holds for $\overline{\Psi} \otimes h^*(\wedge^n\overline{\mathcal{E}}^\vee)(n)$. Therefore the equality in the statement of this theorem follows from our claim before. □

Corollary 6.4. *Let notations and assumptions be as in Theorem 6.3, and let x be any element in $\widehat{K_0}(Z,\mu_n,\emptyset)_\rho$. Then the formula*

$$\begin{aligned} f^Z_{\mu_n *}(i^*x\mid_{X_{\mu_n}} \cdot \sum(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}})) \\ - h_{\mu_n *}(x\mid_{Z_{\mu_n}} \cdot \sum(-1)^k(\overline{\xi}_k\mid_{Z_{\mu_n}})) \\ = \int_{Z_g/Y} T_g(\overline{\xi.})\mathrm{Td}(\overline{Th_g})\mathrm{ch}_g(x) \\ + \int_{X_g/Y} \mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)\mathrm{ch}_g(i^*x) \\ + \int_{X_g/Y} \mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{ch}_g(i^*x)\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g}) \end{aligned}$$

holds in $\widehat{G_0}(Y,\mu_n,\emptyset)_\rho$.

Proof. If $x = \overline{E}$ is an equivariant hermitian vector bundle on Z, then $\overline{\xi.} \otimes \overline{E}$ provides a resolution of $i_*(\overline{\eta}\otimes i^*\overline{E})$. Hence the formula follows from Theorem 6.3 in this case. If $x = \alpha$ is represented by some smooth form, then

$$\begin{aligned} f^Z_{\mu_n *}(i^*x\mid_{X_{\mu_n}} \cdot \sum(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}})) \\ = \int_{Z_g/Y} \mathrm{Td}(Tf_g,\omega_X^Z)\mathrm{Td}_g^{-1}(\overline{F})\mathrm{ch}_g(\overline{\eta})\delta_{X_g}\alpha \end{aligned}$$

and

$$h_{\mu_n *}(x \mid_{Z_{\mu_n}} \cdot \sum(-1)^k(\overline{\xi}_k \mid_{Z_{\mu_n}})) = \int_{Z_g/Y} \mathrm{Td}(\overline{Th_g})\alpha \sum(-1)^k \mathrm{ch}_g(\overline{\xi}_k).$$

Moreover, by the definition of $\mathrm{ch}_g(x)$ we have

$$\int_{Z_g/Y} T_g(\overline{\xi}.)\mathrm{Td}(\overline{Th_g})\mathrm{ch}_g(x) = \int_{Z_g/Y} \mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\delta_{X_g}\mathrm{Td}(\overline{Th_g})\alpha - \int_{Z_g/Y} \sum(-1)^k \mathrm{ch}_g(\overline{\xi}_k)\mathrm{Td}(\overline{Th_g})\alpha$$

and

$$\int_{X_g/Y} \mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)\mathrm{ch}_g(i^*x) = 0.$$

Finally, using the definition of $\widetilde{\mathrm{Td}}$ we compute

$$\begin{aligned}
&\int_{X_g/Y} \mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{ch}_g(i^*x)\widetilde{\mathrm{Td}}((Tf_g, \omega_X^Z), \overline{Th_g} \mid_{X_g}) \\
&= \int_{Z_g/Y} \mathrm{Td}(Tf_g, \omega_X^Z)\mathrm{Td}_g^{-1}(\overline{F})\mathrm{ch}_g(\overline{\eta})\delta_{X_g}\alpha \\
&\qquad - \int_{Z_g/Y} \mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\delta_{X_g}\mathrm{Td}(\overline{Th_g})\alpha.
\end{aligned}$$

Gathering all computations above, we know that the formula still holds for x which is represented by smooth form. Since both two sides are additive, we are done. □

Corollary 6.5. *Let notations and assumptions be as in Theorem 6.3, and let y be any element in $\widehat{K_0}(Z_{\mu_n}, \mu_n, \emptyset)_\rho$. Then the formula*

$$\begin{aligned}
&f^Z_{\mu_n *}(i^*_{\mu_n}y \cdot \sum(-1)^k \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}})) - h_{\mu_n *}(y \cdot \sum(-1)^k(\overline{\xi}_k \mid_{Z_{\mu_n}})) \\
&= \int_{Z_g/Y} T_g(\overline{\xi}.)\mathrm{Td}(\overline{Th_g})\mathrm{ch}_g(y) \\
&\quad + \int_{X_g/Y} \mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)\mathrm{ch}_g(i^*_{\mu_n}y) \\
&\quad + \int_{X_g/Y} \mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{ch}_g(i^*_{\mu_n}y)\widetilde{\mathrm{Td}}((Tf_g, \omega_X^Z), \overline{Th_g} \mid_{X_g})
\end{aligned}$$

holds in $\widehat{G_0}(Y, \mu_n, \emptyset)_\rho$.

Proof. Provided Corollary 6.4, it is enough to prove that for any $y \in \widehat{K_0}(Z_{\mu_n}, \mu_n, \emptyset)_\rho$ there exists an element $x \in \widehat{K_0}(Z, \mu_n, \emptyset)_\rho$ such that $i_Z^* x = y$.

Here i_Z stands for the inclusion $Z_{\mu_n} \hookrightarrow Z$. Actually, set $x = i_{Z*}(\lambda_{-1}^{-1}(\overline{N}^{\vee}_{Z/Z_{\mu_n}}) \cdot y)$, we have

$$i_Z^* x = i_Z^* i_{Z*}(\lambda_{-1}^{-1}(\overline{N}^{\vee}_{Z/Z_{\mu_n}}) \cdot y) = \lambda_{-1}(\overline{N}^{\vee}_{Z/Z_{\mu_n}}) \cdot \lambda_{-1}^{-1}(\overline{N}^{\vee}_{Z/Z_{\mu_n}}) \cdot y = y.$$

This follows from our arithmetic concentration theorem. □

6.3 Proof of the fixed point formula

In this subsection, we provide a complete proof of Theorem 6.1 the singular Lefschetz fixed point formula. Before that, we need to translate Bismut-Ma's immersion formula to an arithmetic G_0-theoretic version. That's the following.

Theorem 6.6. *Let notations and assumptions be as in Section 6.1. Assume that $\overline{\eta}$ is an equivariant hermitian sheaf on X and $\overline{\xi.}$ is a bounded complex of equivariant hermitian vector bundles providing a resolution of $i_*\overline{\eta}$ on Z whose metrics satisfy Bismut assumption (A). Then the equality*

$$\begin{aligned} f_*^Z(\overline{\eta}) - \sum_{j=0}^m (-1)^j h_*(\overline{\xi}_j) = & \int_{X_g/Y} \mathrm{ch}_g(\eta) R_g(N) \mathrm{Td}_g(Tf) \\ & + \int_{Z_g/Y} T_g(\overline{\xi}.) \mathrm{Td}_g(\overline{Th}) \\ & + \int_{X_g/Y} \mathrm{ch}_g(\overline{\eta}) \widetilde{\mathrm{Td}}_g((Tf, \omega_X^Z), \overline{Th}\mid_X) \mathrm{Td}_g^{-1}(\overline{N}) \end{aligned}$$

holds in $\widehat{G_0}(Y, \mu_n, \emptyset)$.

Proof. We first suppose that η and $\xi.$ are all acyclic, then the verification follows rather directly from the generating relations of arithmetic G_0-theory. In fact

$$\begin{aligned} f_*^Z(\overline{\eta}) - \sum_{j=0}^m (-1)^j h_*(\overline{\xi}_j) = & \overline{f_*\eta} - T_g(\omega_X^Z, h^\eta) - (\sum_{j=0}^m (-1)^j (\overline{h_*\xi_j} - T_g(\omega^Z, h^{\xi_j}))) \\ = & \widetilde{\mathrm{ch}}_g(h_*\Xi) - T_g(\omega_X^Z, h^\eta) + \sum_{j=0}^m (-1)^j T_g(\omega^Z, h^{\xi_j}). \end{aligned}$$

And the right-hand side of the last equality is exactly the left-hand side of Bismut-Ma's immersion formula. We emphasize again that to simplify the right-hand side of Bismut-Ma's immersion formula, we have used an Atiyah-Segal-Singer type formula for immersion

$$i_{g*}(\mathrm{Td}_g^{-1}(N) \mathrm{ch}_g(x)) = \mathrm{ch}_g(i_*(x)).$$

To remove the condition of acyclicity, one can use the argument which is essentially the same as in the proof of Theorem 6.3. Since it doesn't use any new techniques, we omit it here. □

Definition 6.7. The inclusion $i : X \hookrightarrow Z$ induces an embedding morphism

$$i_*: \quad \widehat{G_0}(X, \mu_n, \emptyset) \to \widehat{K_0}(Z, \mu_n, N_{g,\mathbb{R}}^\vee \setminus \{0\})$$

which is defined as follows.
(i). For every μ_n-equivariant hermitian sheaf $\overline{\eta}$ on X, suppose that $\overline{\xi.}$ is a resolution of $i_*\overline{\eta}$ on Z whose metrics satisfy Bismut assumption (A), $i_*[\overline{\eta}] = \sum_k (-1)^k[\overline{\xi}_k] + T_g(\overline{\xi.})$.
(ii). For every $\alpha \in \widetilde{\mathcal{U}}(X_{\mu_n}, \emptyset)$, $i_*\alpha = \alpha \mathrm{Td}_g^{-1}(\overline{N})\delta_{X_g}$.

Remark 6.8. Similar to Theorem 5.2 and Lemma 5.3, one can prove that the embedding morphism is a well-defined homomorphism of $R(\mu_n)$-modules.

Proof. (of Theorem 6.1) We first prove that this fixed point formula holds when ω^X is equal to ω_X^Z, namely the Kähler metric on $X(\mathbb{C})$ is induced by the Kähler metric on $Z(\mathbb{C})$. By Theorem 6.6 and Definition 6.7, we have the following equality

$$\begin{aligned} f_*^Z(\overline{\eta}) =& h_* i_*(\overline{\eta}) + \int_{X_g/Y} \mathrm{ch}_g(\eta) R_g(N) \mathrm{Td}_g(Tf) \\ &+ \int_{X_g/Y} \mathrm{ch}_g(\overline{\eta}) \widetilde{\mathrm{Td}}_g((Tf, \omega_X^Z), \overline{Th}\mid_X) \mathrm{Td}_g^{-1}(\overline{N}) \end{aligned}$$

which holds in $\widehat{G_0}(Y, \mu_n, \emptyset)$. Now we claim that for any element $y \in \widehat{K_0}(Z_{\mu_n}, \mu_n, N_{g,\mathbb{R}}^\vee \setminus \{0\})_\rho$, we have

$$h_{\mu_n *}(y) - h_* i_{Z*}(y) = h_{\mu_n *}(y \cdot R_g(N_{Z/Z_{\mu_n}})).$$

Since all morphisms are homomorphisms of $R(\mu_n)$-modules, we can only consider the generators of $\widehat{K_0}(Z_{\mu_n}, \mu_n, N_{g,\mathbb{R}}^\vee \setminus \{0\})$. Indeed, by applying Theorem 6.6 to the closed immersion i_Z, for any equivariant hermitian vector bundle $\overline{E}$ on Z_{μ_n} we have

$$\begin{aligned} h_{\mu_n *}(\overline{E}) - h_* i_{Z*}(\overline{E}) =& \int_{Z_g/Y} \mathrm{ch}_g(E) R_g(N_{Z/Z_{\mu_n}}) \mathrm{Td}_g(Th_g) \\ =& h_{\mu_n *}(\mathrm{ch}_g(E) R_g(N_{Z/Z_{\mu_n}})). \end{aligned}$$

The first equality holds because the exact sequence

$$0 \to \overline{Th_g} \to \overline{Th}\mid_{Z_g} \to \overline{N}_{Z/Z_g} \to 0$$

is orthogonally split on Z_g so that $\widetilde{\mathrm{Td}}_g(\overline{Th_g}, \overline{Th}\mid_{Z_g}) = 0$. The second equality follows from [21, Lemma 7.3] and the fact that $\mathrm{ch}_g(E) R_g(N_{Z/Z_{\mu_n}})$ is dd^c-closed. On the other hand, let α be an element in $\widetilde{\mathcal{U}}(Z_{\mu_n}, N_{g,\mathbb{R}}^\vee \setminus \{0\})$, we have

$$\begin{aligned} h_{\mu_n *}(\alpha) - h_* i_{Z*}(\alpha) =& \int_{Z_g/Y} \alpha \mathrm{Td}_g(\overline{Th_g}) - \int_{Z_g/Y} \alpha \mathrm{Td}_g^{-1}(\overline{N}_{Z/Z_{\mu_n}}) \mathrm{Td}_g(\overline{Th}) \\ =& \int_{Z_g/Y} \alpha \mathrm{Td}_g^{-1}(\overline{N}_{Z/Z_{\mu_n}}) \mathrm{dd}^c \widetilde{\mathrm{Td}}_g(\overline{Th_g}, \overline{Th}\mid_{Z_g}) = 0. \end{aligned}$$

Combing these two computations, we get our claim by linear extension.

Now using arithmetic concentration theorem, we compute

$$\begin{aligned}
h_*i_*(\overline{\eta}) =& h_*i_{Z*}i_{Z*}^{-1}i_*(\overline{\eta})\\
=& h_{\mu_n *}(i_{Z*}^{-1}i_*(\overline{\eta})\cdot(1-R_g(N_{Z/Z_{\mu_n}})))\\
=& h_{\mu_n *}(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee)\cdot i_Z{}^*i_*(\overline{\eta})\cdot(1-R_g(N_{Z/Z_{\mu_n}})))\\
=& h_{\mu_n *}(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee)\cdot\{\sum_k(-1)^k(\overline{\xi}_k\mid_{Z_{\mu_n}})\\
&\qquad\qquad + T_g(\overline{\xi.})\}\cdot(1-R_g(N_{Z/Z_{\mu_n}})))\\
=& h_{\mu_n *}(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee)\cdot\sum_k(-1)^k(\overline{\xi}_k\mid_{Z_{\mu_n}}))\\
&+ h_{\mu_n *}(\mathrm{Td}_g(\overline{N}_{Z/Z_{\mu_n}})T_g(\overline{\xi.}))\\
&- h_{\mu_n *}(\mathrm{Td}_g(N_{Z/Z_{\mu_n}})\sum_k(-1)^k\mathrm{ch}_g(\xi_k)R_g(N_{Z/Z_{\mu_n}})).
\end{aligned}$$

According to Corollary 6.5, by setting $y=\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee)$, we compute

$$\begin{aligned}
&h_{\mu_n *}(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee)\cdot\sum_k(-1)^k(\overline{\xi}_k\mid_{Z_{\mu_n}}))\\
=& f^Z_{\mu_n *}(i_{\mu_n}^*(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee))\cdot\sum(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}}))\\
&-\int_{Z_g/Y}T_g(\overline{\xi.})\mathrm{Td}(\overline{Th_g})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\\
&-\int_{X_g/Y}\mathrm{Td}(Tf_g)\mathrm{Td}_g^{-1}(F)\mathrm{ch}_g(\eta)R(N_g)\mathrm{Td}_g(N_{Z/Z_g})\\
&-\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g})\\
=& f^Z_{\mu_n *}(i_{\mu_n}^*(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee))\cdot\sum(-1)^k\mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta},\overline{\mathcal{O}}_{Z_{\mu_n}}))\\
&-\int_{Z_g/Y}T_g(\overline{\xi.})\mathrm{Td}_g(\overline{Th})-\int_{X_g/Y}\mathrm{Td}_g(Tf)\mathrm{ch}_g(\eta)R(N_g)\\
&-\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g}).
\end{aligned}$$

Here we have used various relations of character forms or characteristic classes arising from the following double complex

$$\begin{array}{ccccccccc}
 & & 0 & & 0 & & 0 & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & (Tf_g, \omega_X^Z) & \longrightarrow & \overline{Th_g} & \longrightarrow & \overline{N}_g & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & (Tf, \omega_X^Z) & \longrightarrow & \overline{Th} & \longrightarrow & \overline{N} & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & (N_{X/X_g}, \omega_X^Z) & \longrightarrow & \overline{N}_{Z/Z_g} & \longrightarrow & \overline{F} & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & & 0 & & 0 & &
\end{array}$$

whose columns are all orthogonally split. Also, for this double complex, one may use Example 2.3 (iv) to compute that

$$\begin{aligned}\widetilde{\mathrm{Td}}_g((Tf,\omega_X^Z),\overline{Th}\mid_X) =& \widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega_X^Z)\mathrm{Td}(\overline{N}_g)\mathrm{Td}(Tf_g,\omega_X^Z) \\ &+ \widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g})\mathrm{Td}_g(\overline{N}_{Z/Z_g}). \end{aligned} \tag{11}$$

We deduce from (11) that

$$\begin{aligned} &\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g((Tf,\omega_X^Z),\overline{Th}\mid_X)\mathrm{Td}_g^{-1}(\overline{N}) \\ =&\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}((Tf_g,\omega_X^Z),\overline{Th_g}\mid_{X_g})\mathrm{Td}_g^{-1}(\overline{N})\mathrm{Td}_g(\overline{N}_{Z/Z_g}) \\ &+\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}})\mathrm{Td}_g^{-1}(\overline{F})\mathrm{Td}(Tf_g,\omega_X^Z). \end{aligned} \tag{12}$$

Moreover, we have

$$\begin{aligned} h_{\mu_n *}(\mathrm{Td}_g(\overline{N}_{Z/Z_{\mu_n}})T_g(\overline{\xi.})) &= \int_{Z_g/Y}T_g(\overline{\xi.})\mathrm{Td}(\overline{Th_g})\mathrm{Td}_g(\overline{N}_{Z/Z_g}) \\ &= \int_{Z_g/Y}T_g(\overline{\xi.})\mathrm{Td}_g(\overline{Th}) \end{aligned} \tag{13}$$

and

$$\begin{aligned} &h_{\mu_n *}(\mathrm{Td}_g(N_{Z/Z_{\mu_n}})\sum_k(-1)^k\mathrm{ch}_g(\xi_k)R_g(N_{Z/Z_{\mu_n}})) \\ =&\int_{Z_g/Y}\mathrm{Td}_g(N_{Z/Z_{\mu_n}})\delta_{X_g}\mathrm{ch}_g(\eta)\mathrm{Td}_g^{-1}(N)R_g(N_{Z/Z_g})\mathrm{Td}(Th_g) \end{aligned}$$

$$
\begin{aligned}
&= \int_{X_g/Y} \mathrm{Td}_g(N_{X/X_g})\mathrm{Td}_g(F)\mathrm{ch}_g(\eta)\mathrm{Td}_g^{-1}(N) \\
&\qquad \cdot [R_g(N_{X/X_g}) + R_g(N) - R(N_g)]\mathrm{Td}(Tf_g)\mathrm{Td}(N_g) \\
&= \int_{X_g/Y} \mathrm{Td}_g(Tf)\mathrm{ch}_g(\eta)[R_g(N_{X/X_g}) + R_g(N) - R(N_g)]. \qquad (14)
\end{aligned}
$$

Gathering (12), (13) and (14) we finally get

$$
\begin{aligned}
f_*^Z(\overline{\eta}) =& f_{\mu_n *}^Z(i_{\mu_n}^*(\lambda_{-1}^{-1}(\overline{N}_{Z/Z_{\mu_n}}^\vee)) \cdot \sum_k (-1)^k \mathrm{Tor}_{\mathcal{O}_Z}^k(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}})) \\
&+ \int_{X_g/Y} \mathrm{Td}(Tf_g, \omega_X^Z)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}}, \omega_X^Z)\mathrm{Td}_g^{-1}(\overline{F}) \\
&- \int_{X_g/Y} \mathrm{Td}_g(Tf)\mathrm{ch}_g(\eta)R_g(N_{X/X_g})
\end{aligned}
$$

which completes the proof of Theorem 6.1 in the case where the Kähler metric on $X(\mathbb{C})$ is induced by the Kähler metric on $Z(\mathbb{C})$.

In general, in analogy with the notation $\widetilde{\mathrm{Td}}(Tf_g, \omega^X, \omega_X^Z)$, we write $\widetilde{\mathrm{Td}}_g(N_{X/X_g}, \omega^X, \omega_X^Z)$ for the secondary characteristic class of the exact sequence

$$
0 \longrightarrow N_{X/X_g} \xrightarrow{\mathrm{Id}} N_{X/X_g} \longrightarrow 0 \longrightarrow 0
$$

where the middle term carries the metric induced by ω_X^Z and the sub term carries the metric induced by ω^X. Similarly, we have the notation $\widetilde{\mathrm{Td}}_g(Tf, \omega^X, \omega_X^Z)$. Then by applying the argument in the proof of (11) to the double complex

$$
\begin{array}{ccccccccc}
 & & 0 & & 0 & & 0 & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & (Tf_g, \omega^X) & \longrightarrow & (Tf_g, \omega_X^Z) & \longrightarrow & 0 & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & (Tf, \omega^X) & \longrightarrow & (Tf, \omega_X^Z) & \longrightarrow & 0 & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & (N_{X/X_g}, \omega^X) & \longrightarrow & (N_{X/X_g}, \omega_X^Z) & \longrightarrow & 0 & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & & 0 & & 0 & &
\end{array}
$$

We get

$$\begin{aligned}\widetilde{\mathrm{Td}}_g(Tf,\omega^X,\omega^Z_X) =&\widetilde{\mathrm{Td}}(Tf_g,\omega^X,\omega^Z_X)\mathrm{Td}_g(N_{X/X_g},\omega^Z_X)\\ &+\widetilde{\mathrm{Td}}_g(N_{X/X_g},\omega^X,\omega^Z_X)\mathrm{Td}(Tf_g,\omega^X).\end{aligned}$$

Moreover, by [30, Proposition 2.8], we obtain that

$$\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^X)=\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^Z_X)+\widetilde{\mathrm{Td}}_g(N_{X/X_g},\omega^X,\omega^Z_X)\mathrm{Td}_g(\overline{F}).$$

With these two comparison formulae, we can compute

$$\begin{aligned}&\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^X)\mathrm{Td}_g^{-1}(\overline{F})\\ &\qquad -\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^Z_X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^Z_X)\mathrm{Td}_g^{-1}(\overline{F})\\ =&\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^X)\mathrm{Td}_g^{-1}(\overline{F})\\ &-\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^Z_X)\mathrm{Td}_g^{-1}(\overline{F})\\ &+\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^Z_X)\mathrm{Td}_g^{-1}(\overline{F})\\ &-\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^Z_X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}},\omega^Z_X)\mathrm{Td}_g^{-1}(\overline{F})\\ =&\int_{X_g/Y}\widetilde{\mathrm{Td}}(Tf_g,\omega^X,\omega^Z_X)\mathrm{ch}_g(\overline{\eta})\\ &\cdot[\mathrm{Td}_g(N_{X/X_g},\omega^Z_X)\mathrm{Td}_g(\overline{F})-\mathrm{Td}_g(\overline{N}_{Z/Z_g})]\mathrm{Td}_g^{-1}(\overline{F})\\ &+\int_{X_g/Y}\mathrm{Td}(Tf_g,\omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(N_{X/X_g},\omega^X,\omega^Z_X)\\ =&\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(Tf,\omega^X,\omega^Z_X)\\ &-\int_{X_g/Y}\widetilde{\mathrm{Td}}(Tf_g,\omega^X,\omega^Z_X)\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\mathrm{Td}_g^{-1}(\overline{F}).\end{aligned}$$

At last, using [21, Lemma 7.3], we get the equality

$$f_*(\overline{\eta})-f_*^Z(\overline{\eta})=\int_{X_g/Y}\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(Tf,\omega^X,\omega^Z_X).$$

Together with the fact that the other two terms have nothing to do with the choice of the metric ω^X, we finally obtain that

$$\begin{aligned} f_*(\overline{\eta}) =& f^Z_{\mu_n *}(i^*_{\mu_n}(\lambda^{-1}_{-1}(\overline{N}^\vee_{Z/Z_{\mu_n}})) \cdot \sum_k (-1)^k \mathrm{Tor}^k_{\mathcal{O}_Z}(i_*\overline{\eta}, \overline{\mathcal{O}}_{Z_{\mu_n}})) \\ &+ \int_{X_g/Y} \mathrm{Td}(Tf_g, \omega^X)\mathrm{ch}_g(\overline{\eta})\widetilde{\mathrm{Td}}_g(\overline{\mathcal{F}}, \omega^X)\mathrm{Td}^{-1}_g(\overline{F}) \\ &- \int_{X_g/Y} \mathrm{Td}_g(Tf)\mathrm{ch}_g(\eta)R_g(N_{X/X_g}) \\ &+ \int_{X_g/Y} \widetilde{\mathrm{Td}}(Tf_g, \omega^X, \omega^Z_X)\mathrm{ch}_g(\overline{\eta})\mathrm{Td}_g(\overline{N}_{Z/Z_g})\mathrm{Td}^{-1}_g(\overline{F}) \end{aligned}$$

which ends the proof of Theorem 6.1. □

Remark 6.9. Let Y be an affine arithmetic scheme Spec(D), and choose ω^X to be the induced Kähler form ω^Z_X. Then the formula in Theorem 6.1 is the content of [25, Conjecture 5.1].

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