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Higher-order spectral shift for pairs of contractions via multiplicative path

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ABSTRACT. Marcantognini and Morán obtained the Koplienko-Neidhardt trace formula in [17] for pairs of contractions and pairs of maximal dissipative operators via multiplicative path. In this article, we prove the existence of higher-order spectral shift functions for pairs of contractions and pairs of maximal dissipative operators via multiplicative path by adapting the argument employed in [17].

CONTENTS

1. Introduction

The spectral shift function (SSF) has become a fundamental object in perturbation theory. The notion of first-order spectral shift function originated from the work of Lifshits on theoretical physics [16], followed by Krein in [13, 15], in which it was shown that for a pair of self-adjoint (not necessarily bounded) operators H and H_0 satisfying $H - H_0 \in \mathcal{B}_1(\mathcal{H})$ (the set of trace class operators on a separable Hilbert space $\mathcal{H}$), there exists a unique real-valued $L^1(\mathbb{R})$- function ξ such that

$$\operatorname{Tr}\{\phi(H) - \phi(H_0)\} = \int_{\mathbb{R}} \phi'(\lambda)\, \xi(\lambda)\, d\lambda, \tag{1}$$

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for a large class of functions ϕ. The function ξ is known as Krein's spectral shift function, and the relation (1) is called Krein's trace formula. A similar result was obtained by Krein in [14] for pair of unitary operators $\{U, U_0\}$ such that $U - U_0 \in \mathcal{B}_1(\mathcal{H})$. For each such pair, there exists a real-valued $L^1([0, 2\pi])$-function ξ, unique modulo an additive constant, such that

$$\operatorname{Tr}\{\phi(U) - \phi(U_0)\} = \int_0^{2\pi} \frac{d}{dt}\{\phi(\mathrm{e}^{it})\}\, \xi(t)\, dt, \tag{2}$$

where ϕ' has an absolutely convergent Fourier series. The original proof of Krein uses analytic function theory, and for various alternative proofs of the formula (1) and (2), we refer to [4, 5, 19, 20, 41]. Moreover, for a description of a wider class of functions for which formulae (1) and (2) hold, we refer to [2, 28]. For a pair of contractions T_1, T_0 with $T_1 - T_0$ trace-class, Neidhardt [22, 23] initiated the study of trace formula, to be followed by others in [1, 9, 18]. In this connection, it is worthwhile to mention that a series of papers by Rybkin [33, 34, 35, 36], where an analogous extension of (1) and (2) in case of contractions was also achieved.

The modified second-order spectral shift function in the case of non-trace class perturbations was introduced by Koplienko in [12]. In 1984, Koplienko also conjectured the existence of the higher order spectral shift measures. In 2013, Potapov, Skripka, and Sukochev affirmatively resolved Koplienko's conjecture in [29] using an important and advanced tool in perturbation theory, namely Multiple Operator Integrals (MOI) and proved the following:

$$\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right) = \int_{\mathbb{R}} f^{(n)}(\lambda)\eta_n(\lambda)d\lambda, \text{ where}$$

$$\mathcal{R}_{H_0,f,n}(V) := f(H_0 + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} f(H_s), \tag{3}$$

for every sufficiently smooth function f, $H_s = H_0 + sV$, $s \in \mathbb{R}$, and $f^{(n)}$ denotes the n-th order derivative of f, where H and H_0 are two self-adjoint operators in a separable Hilbert space $\mathcal{H}$ such that $H - H_0 = V \in \mathcal{B}_n(\mathcal{H})$ (n-th Schatten-von Neumann ideal), and the spectral shift function η_n (of order $n \in \mathbb{N}$) is integrable on $\mathbb{R}$ and depends only on H, H_0, and n. For more on the Koplienko trace formula, we refer to [8, 10, 11, 37] and the references cited therein.

Later, for $n = 2$, many authors studied the above formula (3) for various classes of operators H and H_0 in [11, 24, 27, 32]. In 2014, for general $n(\geq 3) \in \mathbb{N}$, Potapov, Skripka and Sukochev obtained the formula (3) for any pair of contractions U_0 and $U_0 + V$ with the perturbation $V \in \mathcal{B}_n(\mathcal{H})$ via linear path in [30, Theorem 1.3]. In other words, they proved the following result:

Theorem 1.1. *(See* [30, Theorem 1.3]*) Let $n \in \mathbb{N}$, $n \geq 3$. Let U_1 and U_0 be two contractions on a separable Hilbert space $\mathcal{H}$, $V := U_1 - U_0 \in \mathcal{B}_n(\mathcal{H})$ and denote $U_s = U_0 + sV$, $s \in [0, 1]$. Then for any complex polynomial f, $\mathcal{R}_{U_0,f,n}(V) \in$*

$\mathcal{B}_1(\mathcal{H})$ and there exists $L^1(\mathbb{T})$-function $\eta_n = \eta_{n,U_0,V}$ such that

$$\mathrm{Tr}\left(\mathcal{R}_{U_0,f,n}(V)\right) = \int_{\mathbb{T}} f^{(n)}(z)\eta_n(z)dz. \tag{4}$$

Furthermore, for every given $\epsilon > 0$, the function η_n satisfying (4) *can be chosen so that $\|\eta_n\|_1 \leq (1+\epsilon)c_n\|V\|_n^n$, where c_n is some constant.*

Going further, in 2016, for general $n \in \mathbb{N}$ with $n \geq 2$, Potapov, Skripka and Sukochev established the formula (3) for the couple of unitaries U_0 and $U_1 = e^{iA}U_0$ with the perturbation $A = A^* \in \mathcal{B}_n(\mathcal{H})$ via multiplicative path in [31, Theorem 4.1] corresponding to the class

$$\mathcal{G}_n(\mathbb{T}) := \Big\{f(z) = \sum_{k=n}^{\infty} \hat{f}(k)z^k \in C(\mathbb{T}) : \sum_{k=n}^{\infty} |\hat{f}(k)|k^n < \infty\Big\},$$

where $\{\hat{f}(k) : k \in \mathbb{Z}\}$ are the Fourier coefficients of f and $C(\mathbb{T})$ is the Banach space of all continuous functions on $\mathbb{T}$ with the standard norm. Later, in 2017, Skripka [38, Theorem 4.4] extends the result of [31, Theorem 4.1] established for $n \geq 2$ and f such that $f^{(n)}$ is given by an absolutely convergent Taylor series, that is, for the class

$$\mathcal{F}_n(\mathbb{T}) := \Big\{f(z) = \sum_{k=-\infty}^{\infty} \hat{f}(k)z^k \in C^n(\mathbb{T}) : \sum_{k=-\infty}^{\infty} |k|^n|\hat{f}(k)| < \infty\Big\},$$

where $C^n(\mathbb{T})$ is the collection of all n-times continuously differentiable functions on $\mathbb{T}$ and $f^{(n)}$ denotes the n-th order derivative of the function $f \in C^n(\mathbb{T})$. More precisely, Skripka obtained the following result, and it will be useful to achieve our main results in later sections:

Theorem 1.2. *(See* [38, Theorem 4.4]*) Let $n \in \mathbb{N}$, $n \geq 2$. Let U_0 be a unitary operator, $A = A^* \in \mathcal{B}_n(\mathcal{H})$ and denote $U_s = e^{isA}U_0$, $s \in [0,1]$. Then, for any $f \in \mathcal{F}_n(\mathbb{T})$, $\mathcal{R}_{U_0,f,n}(V) \in \mathcal{B}_1(\mathcal{H})$ and there exists a constant c_n and a function $\eta_n = \eta_{n,U_0,A} \in L^1([0,2\pi])$ satisfying $\|\eta_n\|_1 \leq c_n\|A\|_n^n$ such that*

$$\mathrm{Tr}\left\{f(U_1) - f(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0} f(U_s)\right\} = \int_0^{2\pi} f^{(n)}(e^{it})\eta_n(t)dt.$$

In this direction of studies, Marcantognini and Morán obtained the Koplienko-Neidhardt trace formula (second order trace formula) for pairs of contraction operators and pairs of maximal dissipative operators via multiplicative path in [17]. The present article aims to prove a higher-order version of the Koplienko-Neidhardt trace formula for pairs of contractions and pairs of maximal dissipative operators via multiplicative path by adapting the method developed for the second-order trace formula in [17]. The novelty of our results is that the extension is natural in comparison with the known higher-order trace formulas for unitary and self-adjoint operators. Moreover, the importance

of our work lies in the fact that our results provide some new addition to the theory of spectral shift functions. One of the major ingredients to prove our main result is the higher-order trace formulas for unitary operators, namely Theorem 1.2. We have adapted the method applied in [17] and modified it appropriately to obtain our main results in this article. The major tools required to achieve our results are the Schäffer matrix unitary dilation and the Cayley transformation. In other words, the transference of the trace formulas from unitary to contractive operators is made by means of the dilation theory, and the transference from the contractive to dissipative operators is made with the help of the Cayley transform as done in [17]. More precisely, the following are the major contributions of this article:

- First, we prove a higher-order version of [17, Theorem 2.1]. In other words, we consider a pair (T, V), where V is a unitary operator and T is a contraction on $\mathscr{H}$. Then we prove a higher-order version of the Koplienko-Neidhardt trace formula via multiplicative path corresponding to the pair (T, V) under some additional hypotheses (see Theorem 3.2) by using dilation theory and applying Theorem 1.2.
- Next, we obtain a higher-order version of [17, Theorem 2.3]. More precisely, we prove a higher-order version of the Koplienko-Neidhardt trace formula via multiplicative path for pairs of contractions (T_0, T_1) (see Theorem 4.1) by using our Theorem 3.2.
- At the end, we prove a higher-order version of [17, Theorem 2.3]. In other words, as an application of our Theorem 4.1 for pairs of contractions, we obtain a higher-order analog of the Koplienko-Neidhardt trace formula via multiplicative path for pairs of maximal dissipative operators (see Theorem 5.2).

The major difficulties we face in extending the results of [17] to higher-order are as follows:

- Obtain a precise expression of the k-order derivatives $\dfrac{d^k}{ds^k}\Big|_{s=0}\{(V_s)^n\}$, and $\dfrac{d^k}{ds^k}\Big|_{s=0}\{(T_s)^n\}$, which we are able to overcome due to [39, Theorem 5.3.4](see (18), (19)).
- Secondly, to show $P_{\mathscr{H}}X_r\Big|_{\mathscr{H}} = Y_r$ and

$$P_{\mathscr{F}\ominus\mathscr{H}}X_r\Big|_{\mathscr{F}\ominus\mathscr{H}} = P_{\mathbf{H}^2_{\mathscr{D}_T}(\mathbb{D})}X_rP_{\mathbf{H}^2_{\mathscr{D}_{T^*}}(\mathbb{D})}\Big|_{\mathscr{F}\ominus\mathscr{H}}$$

  for $r \geq 2$, which we are able to complete by rigorously analyzing the block matrix representations of the corresponding operators and shifting the projections from left to right accordingly (see (21), (22), (37), (38), and (39)).

The rest of the paper is organized as follows: Section 2 deals with some essential preliminaries, which will be useful in later sections. In Section 3, we prove the

higher-order analog of the Koplienko-Neidhardt trace formula corresponding to the pair (T, V) via multiplicative path, where V is a unitary operator and T is a contraction on $\mathcal{H}$. Section 4 is devoted to obtaining a higher-order version of the Koplienko-Neidhardt trace formula for pairs of contractions via multiplicative path. Consequently, in Section 5, we prove the trace formula for pairs of maximal dissipative operators.

2. Preliminaries

Notations: Here, $\mathcal{H}$ will denote the separable infinite dimensional Hilbert space we work in; $\mathcal{B}(\mathcal{H})$, $\mathcal{B}_1(\mathcal{H})$, $\mathcal{B}_2(\mathcal{H})$, $\mathcal{B}_n(\mathcal{H})$ the set of bounded, trace class, Hilbert-Schmidt class, Schatten-n class operators in $\mathcal{H}$ respectively with $\|\cdot\|$, $\|\cdot\|_1$, $\|\cdot\|_2$, $\|\cdot\|_n$ as the associated norms. Given $T \in \mathcal{B}(\mathcal{H})$, we denote its kernel by $\mathrm{Ker}(T)$, its range by $\mathrm{Ran}(T)$ and its spectrum by $\sigma(T)$, and let $\mathrm{Dom}(A)$, $\mathrm{Tr}(A)$ be the domain of the operator A and the trace of a trace class operator A respectively. Also, $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{R}$, and $\mathbb{C}$ denote the collection of natural, integer, real, and complex numbers, respectively. Furthermore, $\mathbb{D}$ stands for the open unit disk in the complex plane $\mathbb{C}$ and $\mathbb{T}$ for the unit circle in $\mathbb{C}$, hence $\mathbb{D} := \{|z| < 1,\ z \in \mathbb{C}\}$ and $\mathbb{T} := \{|z| = 1,\ z \in \mathbb{C}\}$. Further, given a closed subspace $\mathcal{M}$ of $\mathcal{H}$, $P_{\mathcal{M}}$ denotes the orthogonal projection of $\mathcal{H}$ onto $\mathcal{M}$.

Recall that $\mathcal{H}$-valued Hardy space over the unit disc $\mathbb{D}$ in $\mathbb{C}$ is denoted by $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ and defined by

$$\mathbf{H}^2_{\mathcal{H}}(\mathbb{D}) := \left\{ f(z) = \sum_{k=0}^{\infty} a_k z^k : \|f\|^2_{\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})} := \sum_{k=0}^{\infty} \|a_k\|^2_{\mathcal{H}} < \infty,\ z \in \mathbb{D},\ a_k \in \mathcal{H} \right\}. \quad (5)$$

Recall that the shift operator on the Hardy space $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ is denoted by $S_{\mathcal{H}}$ and is defined by $(S_{\mathcal{H}} f)(z) := zf(z)$, $f \in \mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$, $z \in \mathbb{D}$. It is easy to check that $S_{\mathcal{H}}$ is an isometry on $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ and $S_{\mathcal{H}} S^*_{\mathcal{H}} = I - P_{\mathcal{H}}$, where $P_{\mathcal{H}}$ is the orthogonal projection of $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ onto $\mathcal{H}$ (that is, by identifying $\mathcal{H}$ as $\mathcal{H}$-valued constant functions). For more on vector-valued Hardy space, we refer to [25, 26].

Let $T \in \mathcal{B}(\mathcal{H})$ be a contraction, that is $\|T\| \leq 1$. Then the defect operator of T is denoted by D_T and defined by $D_T := (1 - T^*T)^{1/2}$. Moreover, $\mathcal{D}_T := \overline{\mathrm{Ran}(D_T)}$ is known as the corresponding defect space of T. Recall that the minimal unitary dilation of a contraction T is a unitary operator $U_T : \mathcal{F} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \to \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ such that $T^n = P_{\mathcal{H}} U_T^n|_{\mathcal{H}}$ and $T^{*^n} = P_{\mathcal{H}} U_T^{-n}|_{\mathcal{H}}$ for $n \in \mathbb{N}$, and $\mathcal{F}$ is the smallest Hilbert space containing the subspaces $U_T^n \mathcal{H}$ for all $n \in \mathbb{Z}$. Furthermore, the block matrix (Schäffer matrix) representation of U_T is as follows:

$$U_T = \begin{bmatrix} S^*_{\mathcal{D}_{T^*}} & 0 & 0 \\ D_{T^*} P_{\mathcal{D}_{T^*}} & T & 0 \\ -T^* P_{\mathcal{D}_{T^*}} & D_T & S_{\mathcal{D}_T} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \longrightarrow \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}, \quad (6)$$

where $S_{\mathcal{D}_T}$ and $S_{\mathcal{D}_{T^*}}$ are the shift operator on $\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ and $\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})$ respectively and $P_{\mathcal{D}_{T^*}}$ is the orthogonal projection from $\mathcal{F}$ onto $\mathcal{D}_{T^*} \oplus \mathbf{0} \oplus \mathbf{0} \equiv \mathcal{D}_{T^*}$. Given a pair of contractions (T_0, T) on $\mathcal{H}$, we denote by $U_{T_0,T}$ the extension of T_0 to the minimal dilation space $\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ of T and the block matrix representation of $U_{T_0,T}$ is given by

$$U_{T_0,T} := \begin{bmatrix} S^*_{\mathcal{D}_{T^*}} & 0 & 0 \\ 0 & T_0 & 0 \\ -V_T^* P_{\mathcal{D}_{T^*}} & 0 & S_{\mathcal{D}_T} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \longrightarrow \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}. \tag{7}$$

For more on dilation theory we refer to [21]. Let $\phi \in \mathcal{F}_n(\mathbb{T})$ be such that $\phi(e^{it}) = \sum_{k=-\infty}^{\infty} \hat{\phi}(k) e^{ikt}$. Next we introduce the functions, namely $\phi_+(e^{it}) = \sum_{k=0}^{\infty} \hat{\phi}(k) e^{ikt}$ and $\phi_-(e^{it}) = \sum_{k=1}^{\infty} \hat{\phi}(-k) e^{ikt}$. Then $\phi(e^{it}) = \phi_+(e^{it}) + \phi_-(e^{-it})$ and $\phi_\pm \in \mathcal{F}_n(\mathbb{T})$. Now for a given contraction T on $\mathcal{H}$, we set

$$\phi_+(T) = \sum_{k=0}^{\infty} \hat{\phi}(k) T^k, \ \phi_-(T) = \sum_{k=1}^{\infty} \hat{\phi}(-k) {T^*}^k, \text{ and } \phi(T) = \phi_+(T) + \phi_-(T). \tag{8}$$

3. Higher-order Trace formula for pair of contractive operators with one of them unitary

In this section, we prove the higher-order version of the Koplienko- Neidhardt trace formula via multiplicative path for a pair (T, V), where T is a contraction and V is a unitary operator on $\mathcal{H}$ such that $T - V \in \mathcal{B}_n(\mathcal{H})$. To proceed further, we need the following auxiliary lemma to obtain our main result in this section. Note that Lemma 3.1 below is available in [39] (see Theorem 5.3.4) in the case when U is a unitary operator, and the expression of the k-th order Gâteaux derivative of $f(U_t)$ is given in terms of multiple operator integral, where f belongs to the Besov space. On the other hand, in our case, U is a contraction, and f is a polynomial. Nevertheless, by simply mimicking the proof of Theorem 5.3.4 in [39], one can obtain the following Lemma 3.1, and hence the detailed proof is left to the reader.

Lemma 3.1. *Let $p(z) = z^n$, $z \in \mathbb{T}$ and $n \in \mathbb{N}$, let $A \in \mathcal{B}(\mathcal{H})$ be a self-adjoint operator and let $U \in \mathcal{B}(\mathcal{H})$. Set $U_t = e^{itA}U$, $t \in \mathbb{R}$. Then for all $1 \leq k \leq n-1$, we have*

$$\frac{d^k}{dt^k}\Big|_{t=s} \{U_t^n\} = \sum_{r=1}^{k} \sum_{\substack{l_1+l_2+\cdots+l_r=k \\ l_1,l_2,\ldots,l_r \geq 1}} \frac{k!}{l_1! \cdots l_r!}$$

$$\times\left[\sum_{\substack{\alpha_0+\alpha_1+\cdots+\alpha_r=n-r\\ \alpha_0,\alpha_1,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0}W_s^{l_1}U_s^{\alpha_1}\cdots W_s^{l_r}U_s^{\alpha_r}\right], \tag{9}$$

where $W_s^l=\left((iA)^l e^{isA}U\right)$, $l\in\mathbb{N}$.

Now we are in a position to state and prove our main result in this section.

Theorem 3.2. *Let $n\in\mathbb{N}$. Let T and V be two contractions in $\mathcal{H}$ such that*

(i) $V^*V=VV^*=I$, and $\dim(\ker T)=\dim(\ker T^*)$,
(ii) $T-V\in\mathcal{B}_n(\mathcal{H})$, and $(I-T^*T)^{1/2}\in\mathcal{B}_n(\mathcal{H})$.

Let $T=V_T|T|$ be the polar decomposition of T, where V_T is a partial isometry on $\mathcal{H}$ and $|T|=(T^*T)^{1/2}$. Set $\mathcal{L}:=\begin{bmatrix} TV^* & -D_{T^*}V_T\big|_{\mathcal{D}_T}\\ D_TV^* & T^*V_T\big|_{\mathcal{D}_T}\end{bmatrix}:\begin{bmatrix}\mathcal{H}\\ \\ \mathcal{D}_T\end{bmatrix}\longrightarrow\begin{bmatrix}\mathcal{H}\\ \\ \mathcal{D}_T\end{bmatrix}$. Then $\mathcal{L}$ is a unitary operator on $\mathcal{H}\oplus\mathcal{D}_T$ and, hence there exists a unique self-adjoint operator $L\in\mathcal{B}_n(\mathcal{H}\oplus\mathcal{D}_T)$ with $\sigma(L)\subseteq(-\pi,\pi]$ such that $\mathcal{L}=e^{iL}$. Furthermore, if we denote $V_s:=P_{\mathcal{H}}e^{isL}V$, $s\in[0,1]$, then for $\phi\in\mathcal{F}_n(\mathbb{T})$,

$$\left\{\phi(T)-\phi(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\}\in\mathcal{B}_1(\mathcal{H}), \tag{10}$$

and there exists an $L^1([0,2\pi])$-function ξ_n depend only on n,T and V such that

$$\mathrm{Tr}\left\{\phi(T)-\phi(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\}=\int_0^{2\pi}\phi^{(n)}(e^{it})\xi_n(t)dt. \tag{11}$$

Proof. For $n=1,2$, the property (10) and the trace formula (11) were established in [22, Section 2] and [17, Theorem 2.1]. Now we prove the theorem for $n\geq 3$. Let $U_1:=U_T$ be the corresponding minimal unitary dilation of T on $\mathcal{F}=\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})\oplus\mathcal{H}\oplus\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$. Given that $T=V_T|T|$ is the polar decomposition of T, where $|T|=(T^*T)^{1/2}$ and V_T is an isometry from $\overline{Ran(T^*)}$ onto $\overline{Ran(T)}$. Therefore by using the hypothesis $\dim(\ker T)=\dim(\ker T^*)$, we can extend V_T to a unitary operator on the full space $\mathcal{H}$. Going further, we need the following useful relations obtained in [17]

$$\begin{aligned}&V_TD_T=D_{T^*}V_T,\ (1-|T|)=(1+|T|)^{-1}(1-T^*T),\text{ and}\\ &V_T-T=V_T(1-|T|).\end{aligned} \tag{12}$$

Let $U_0:=U_{V,T}:\mathcal{F}\to\mathcal{F}$. Now by using the relations listed in (12) along with the hypothesis (ii) we conclude $U_1-U_0\in\mathcal{B}_n(\mathcal{F})$. Thus, we have a pair (U_1,U_0) of unitary operators on $\mathcal{F}$. By a similar computations as done in the proof of [17, Theorem 2.1], we get a self-adjoint operator $A\in\mathcal{B}_n(\mathcal{F})$ such that $U_1=e^{iA}U_0$

and the block matrix representation of A with respect to the decomposition $\mathcal{F} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus (\mathcal{H} \oplus \mathcal{D}_T) \oplus S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ is the following:

$$A := \begin{bmatrix} 0 & 0 & 0 \\ 0 & L & 0 \\ 0 & 0 & 0 \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}. \tag{13}$$

Therefore the pair (U_1, U_0) satisfies the hypothesis of Theorem 1.2 and hence for any $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\left\{\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(U_s)\right\} \in \mathcal{B}_1(\mathcal{H}), \tag{14}$$

and there exists an $L^1([0, 2\pi])$-function $\eta_n = \eta_{n,U_0,A}$ such that

$$\mathrm{Tr}\left\{\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(U_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it})\eta_n(t)dt, \tag{15}$$

where $U_s = e^{isA}U_0,\ s \in [0, 1]$. Our next aim is to show that for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\begin{aligned} &\mathrm{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\} \\ =&\mathrm{Tr}\left\{\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(U_s)\right\}, \end{aligned} \tag{16}$$

where

$$V_s := P_{\mathcal{H}}e^{isA}U_0\Big|_{\mathcal{H}} = P_{\mathcal{H}}e^{isL}V,\ s \in [0, 1]. \tag{17}$$

To this end, we first deal with the monomials, that is functions like $\phi_q(z) = z^q,\ z \in \mathbb{T}$ and $q \in \mathbb{Z}$. Now if $q \in \mathbb{N}$, then by using Lemma 3.1, we conclude for $1 \le k \le n-1$ that

$$\begin{aligned} \frac{d^k}{ds^k}\Big|_{s=0}\{\phi_q(U_s)\} = \sum_{r=1}^{k} \sum_{\substack{\alpha_0+\cdots+\alpha_r=q-r \\ \alpha_0,\ldots,\alpha_r\ge 0}} \sum_{\substack{l_1+\cdots+l_r=k \\ l_1,\ldots,l_r\ge 1}} \frac{k!}{l_1!\cdots l_r!} U_0^{\alpha_0}((iA)^{l_1}U_0)U_0^{\alpha_1} \\ \cdots((iA)^{l_r}U_0)U_0^{\alpha_r}, \end{aligned} \tag{18}$$

and

$$\begin{aligned} \frac{d^k}{ds^k}\Big|_{s=0}\{\phi_q(V_s)\} = \sum_{r=1}^{k} \sum_{\substack{\alpha_0+\cdots+\alpha_r=q-r \\ \alpha_0,\ldots,\alpha_r\ge 0}} \sum_{\substack{l_1+\cdots+l_r=k \\ l_1,\ldots,l_r\ge 1}} \frac{k!}{l_1!\cdots l_r!} V^{\alpha_0}P_{\mathcal{H}}((iL)^{l_1}V) \\ \times V^{\alpha_1}\cdots P_{\mathcal{H}}((iL)^{l_r}V)V^{\alpha_r}. \end{aligned} \tag{19}$$

To complete the proof of this theorem we need the following essential lemma in the sequel.

Lemma 3.3. *Assume notations and hypotheses of the above Theorem* 3.2*. Let* $U_1 := U_T$ *and* $U_0 = U_{T_0,T}$*. Let*

$$\begin{aligned}
&\mathcal{F} := \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}),\ X_0 := U_1^n - U_0^n,\ Y_0 := T^n - V^n,\\
&X_r := U_0^{\alpha_0}((iA)^{l_1}U_0)\,U_0^{\alpha_1}\cdots((iA)^{l_r}U_0)U_0^{\alpha_r},\ \textit{and}\\
&Y_r := V^{\alpha_0}P_{\mathcal{H}}((iL)^{l_1}V)V^{\alpha_1}\cdots V^{\alpha_{r-1}}P_{\mathcal{H}}((iL)^{l_r}V)V^{\alpha_r},
\end{aligned}$$

where A, L *are given in* (13)*,* $\alpha_j \geq 0$ *for* $0 \leq j \leq r$*, and* $l_{j'} \geq 1$ *for* $1 \leq j' \leq r$ *, and* $r \geq 1$*. Then for every integer* $r \geq 0$*,*

(i) $P_{\mathcal{H}}X_r\Big|_{\mathcal{H}} = Y_r$.

(ii) $P_{\mathcal{F}\ominus\mathcal{H}}X_r\Big|_{\mathcal{F}\ominus\mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})}X_rP_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\Big|_{\mathcal{F}\ominus\mathcal{H}}$.

Proof. For $r = 0, 1$, it was obtained in the proof of [17, Theorem 2.1] that

$$P_{\mathcal{H}}X_r\Big|_{\mathcal{H}} = Y_r. \tag{20}$$

For $r \geq 2$, by analyzing the block matrix representations (6), (7) and (13) of U_1, U_0 and A respectively, we conclude

$$\begin{aligned}
P_{\mathcal{H}}X_r\Big|_{\mathcal{H}} =& P_{\mathcal{H}}U_0^{\alpha_0}((iA)^{l_1}U_0)U_0^{\alpha_1}\cdots((iA)^{l_r}U_0)U_0^{\alpha_r}\Big|_{\mathcal{H}}\\
=& P_{\mathcal{H}}U_0^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_T}U_0)U_0^{\alpha_1}P_{\mathcal{H}\oplus\mathcal{D}_T}\\
&\cdots U_0^{\alpha_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_T}U_0)U_0^{\alpha_r}\Big|_{\mathcal{H}}\\
=& V^{\alpha_0}P_{\mathcal{H}}((iL)^{l_1}V)V^{\alpha_1}\cdots V^{\alpha_{r-1}}P_{\mathcal{H}}((iL)^{l_r}V)V^{\alpha_r} = Y_r.
\end{aligned} \tag{21}$$

On the other hand, for $r = 0, 1$, it was obtained in the proof of [17, Theorem 2.1] that

$$P_{\mathcal{F}\ominus\mathcal{H}}X_r\Big|_{\mathcal{F}\ominus\mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})}X_rP_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\Big|_{\mathcal{F}\ominus\mathcal{H}}.$$

For $r \geq 2$, by analyzing the structures of U_1, U_0, and A as in (6), (7), and (13) respectively we get

$$\begin{aligned}
P_{\mathcal{F}\ominus\mathcal{H}}X_r\Big|_{\mathcal{F}\ominus\mathcal{H}} =& P_{\mathcal{F}\ominus\mathcal{H}}U_0^{\alpha_0}((iA)^{l_1}U_0)U_0^{\alpha_1}\cdots((iA)^{l_r}U_0)U_0^{\alpha_r}\Big|_{\mathcal{F}\ominus\mathcal{H}}\\
=& P_{\mathcal{F}\ominus\mathcal{H}}U_0^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_T}U_0)U_0^{\alpha_1}\\
&\cdots P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_T}U_0)U_0^{\alpha_r}\Big|_{\mathcal{F}\ominus\mathcal{H}}\\
=& P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})}U_0^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_T}U_0)U_0^{\alpha_1}\\
&\times\cdots\times P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_T}U_0)U_0^{\alpha_r}P_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\Big|_{\mathcal{F}\ominus\mathcal{H}}.
\end{aligned} \tag{22}$$

□

Continue of the proof of Theorem 3.2: Therefore using Lemma 3.3 (i), from (18) and (19) we conclude that

$$\begin{aligned}&\phi_q(T)-\phi_q(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(V_s)\\&=P_{\mathscr{H}}\left(\phi_q(U_1)-\phi_q(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(U_s)\right)\Bigg|_{\mathscr{H}},\end{aligned}\tag{23}$$

for all $q\in\mathbb{N}$. For $q\in\mathbb{Z}$, $q<0$, recall that $T^q=T^{*-q}$ for a given contraction T (see (8)). Therefore using the facts

$$\begin{aligned}\frac{d^k}{ds^k}\Big|_{s=0}\{\phi_q(U_s)\}&=\left(\frac{d^k}{ds^k}\Big|_{s=0}\{\phi_{-q}(U_s)\}\right)^* \text{ and}\\ \frac{d^k}{ds^k}\Big|_{s=0}\{\phi_q(V_s)\}&=\left(\frac{d^k}{ds^k}\Big|_{s=0}\{\phi_{-q}(V_s)\}\right)^*,\end{aligned}\tag{24}$$

and applying Lemma 3.1 together with the similar arguments as above, we also conclude that for $q\in\mathbb{Z}$ and $q<0$, (23) holds good. Similarly, (23) also holds good for $q\in\mathbb{Z},\ q<0$. Therefore

$$\left\{\phi_q(T)-\phi_q(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(V_s)\right\}\in\mathcal{B}_1(\mathscr{H}),$$

and

$$\begin{aligned}&\mathrm{Tr}\left\{\phi_q(T)-\phi_q(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(V_s)\right\}\\&=\mathrm{Tr}\left\{P_{\mathscr{H}}\left(\phi_q(U_1)-\phi_q(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(U_s)\right)\Bigg|_{\mathscr{H}}\right\},\quad\forall q\in\mathbb{Z}.\end{aligned}\tag{25}$$

Again using Lemma 3.3 (ii), we conclude that the operator

$$P_{\mathscr{F}\ominus\mathscr{H}}\left(\phi_q(U_1)-\phi_q(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(U_s)\right)\Bigg|_{\mathscr{F}\ominus\mathscr{H}}$$

maps $\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})\oplus\mathbf{0}\oplus\mathbf{0}$ to $\mathbf{0}\oplus\mathbf{0}\oplus\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ for $q\in\mathbb{N}$. These observations immediately yield that

$$\mathrm{Tr}\left\{P_{\mathscr{F}\ominus\mathscr{H}}\left(\phi_q(U_1)-\phi_q(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_q(U_s)\right)\Bigg|_{\mathscr{F}\ominus\mathscr{H}}\right\}=0,\tag{26}$$

for all $q \in \mathbb{N}$. Now by considering the pair (T^*, V^*) instead of (T, V) and repeating the similar calculations as above we conclude that (26) also holds for $q \in \mathbb{Z},\ q < 0$. Therefore combining equations (25) and (26) together with the last line of argument, we conclude

$$\begin{aligned}&\operatorname{Tr}\left\{\phi_q(T) - \phi_q(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(V_s)\right\} \\ =&\operatorname{Tr}\left\{\phi_q(U_1) - \phi_q(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(U_s)\right\}\end{aligned} \tag{27}$$

for all $q \in \mathbb{Z}$. Let $\phi(z) = \sum_{k=-\infty}^{\infty} \hat{\phi}(k) z^k \in \mathcal{F}_n(\mathbb{T})$, and hence $\sum_{k=-\infty}^{\infty} |k|^n |\hat{\phi}(k)| < \infty$. Let $N \in \mathbb{N}$, and let $\phi_N(z) = \sum_{k=-N}^{N} \hat{\phi}(k) z^k$. Then we have the following integral representation

$$\begin{aligned}&\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(U_s) \\ =&\frac{1}{(n-1)!} \int_0^1 (1-t)^{(n-1)} \frac{d^n}{ds^n}\Big|_{s=t} \phi(U_s)\, dt,\end{aligned} \tag{28}$$

where the integral converges in the operator norm. The above representation (28) of the n-th order Taylor remainder is transferred from the analogous representation for scalar functions via the application of bounded linear functionals from $\big(\mathcal{B}(\mathscr{H})\big)^*$ (see, e.g., [31, Equation (4.2)], [40, Theorem 1.43, Corollary 1.45]). Therefore, it follows form (18) and (24) that

$$\begin{aligned}
&\left\|\phi(U_1)-\phi(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(U_s)\right\|_1\\
&\leq \frac{1}{(n-1)!}\int_0^1 (1-t)^{(n-1)}\left\|\frac{d^n}{ds^n}\Big|_{s=t}\phi(U_s)\right\|_1 dt\\
&\leq n^n\left(\sum_{j=-\infty}^{\infty}|j|^n|\hat{\phi}(j)|\right)\|A\|_n^n<\infty,
\end{aligned}$$

which further implies

$$\begin{aligned}
\lim_{N\to\infty}\Bigg\|&\left\{\phi_N(U_1)-\phi_N(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_N(U_s)\right\}\\
&-\left\{\phi(U_1)-\phi(U_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(U_s)\right\}\Bigg\|_1\\
=\ &0. \qquad (29)
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
\lim_{N\to\infty}\Bigg\|&\left\{\phi_N(T)-\phi_N(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi_N(V_s)\right\}\\
&-\left\{\phi(T)-\phi(V)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\}\Bigg\|_1\\
=\ &0. \qquad (30)
\end{aligned}$$

Therefore combining (27), (29) and (30), we have the trace equality (16). Finally the conclusion of the theorem follows by combining equations (15) and (16). This completes the proof.

□

4. Higher-order Trace formula for pair of contractions

In the previous section, we discuss the trace formula for pairs of contractions (T,V) assuming that V is unitary. In this section, we remove the assumption on V. In other words, we prove the trace formula for pairs of contractions (T_0,T_1) on $\mathcal{H}$. The technique involved here is standard and similar to the idea mentioned in [17] with an appropriate modification, that means first we dilate (T_0,T_1) to a pair of contractions (T,V) with V is a unitary operator on the bigger space $\mathcal{F}$ containing $\mathcal{H}$ as a subspace and then use the existing trace formula

for the pair (T, V) obtained in our last section to get the required trace formula in this section. The following is the main result in this section.

Theorem 4.1. *Let $n \in \mathbb{N}$. Let T_0 and T_1 be two contractions in $\mathscr{H}$ such that*

(i) $\dim(\ker T_0) = \dim(\ker T_0^*)$, *and* $\dim(\ker T_1) = \dim(\ker T_1^*)$,

(ii) $T_1 - T_0 \in \mathcal{B}_n(\mathscr{H})$, *and* $(I - T_j^* T_j)^{1/2} \in \mathcal{B}_n(\mathscr{H})$ *for* $j = 0, 1$.

Let $T_j = V_{T_j}|T_j|$ be the polar decomposition of T_j, where V_{T_j} is a partial isometry on $\mathscr{H}$ and $|T_j| = (T_j^* T_j)^{1/2}$ for $j = 0, 1$. Set

$$\mathcal{M} := \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & T_1 T_0^* & T_1 D_{T_0} P_{\mathcal{D}_{T_0}} & -D_{T_1^*} V_{T_1} \\ 0 & -V_{T_0}^* D_{T_0^*} & |T_0| P_{\mathcal{D}_{T_0}} + (I - P_{\mathcal{D}_{T_0}}) & 0 \\ 0 & D_{T_1} T_0^* & D_{T_1} D_{T_0} P_{\mathcal{D}_{T_0}} & T_1^* V_{T_1} \end{bmatrix} :$$
$$\begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}.$$

Then $\mathcal{M}$ is a unitary operator on $\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathscr{H} \oplus \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \oplus \mathcal{D}_{T_1} = \mathscr{F} \oplus \mathcal{D}_{T_1}$ and hence there exists a unique self-adjoint operator $M \in \mathcal{B}_n(\mathscr{F} \oplus \mathcal{D}_{T_1})$ with $\sigma(M) \subseteq (-\pi, \pi]$ such that $\mathcal{M} = e^{iM}$. Furthermore, if we denote

$$T_s = P_{\mathscr{H}} e^{isM} \begin{bmatrix} 0 \\ T_0 \\ D_{T_0} \\ 0 \end{bmatrix} : \mathscr{H} \to \mathscr{H}, \ s \in [0, 1], \tag{31}$$

then for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\left\{ \phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s) \right\} \in \mathcal{B}_1(\mathscr{H}), \tag{32}$$

and there exists an $L^1([0, 2\pi])$-function ξ_n depend only on n, T_1 and T_0 such that

$$\mathrm{Tr}\left\{ \phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s) \right\} = \int_0^{2\pi} \phi^{(n)}(e^{it}) \xi_n(t) dt. \tag{33}$$

The following lemma is essential to prove Theorem 4.1.

Lemma 4.2. *Assume notations and hypotheses of the above Theorem* 4.1. *Let $T := U_{T_1, T_0}, V := U_{T_0}$ and $\mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathscr{H} \oplus \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})$. Let*

$$X_0 := T^n - V^n, Y_0 := T_1^n - T_0^n,$$
$$X_r := V^{\alpha_0} P_{\mathscr{F}} \left((iM)^{l_1} V \right) V^{\alpha_1} \cdots P_{\mathscr{F}} \left((iM)^{l_r} V \right) V^{\alpha_r},$$

$$Y_r := {T_0}^{\alpha_0} P_{\mathscr{H}} \left((iM)^{l_1} W\right) {T_0}^{\alpha_1} \cdots P_{\mathscr{H}} \left((iM)^{l_r} W\right) {T_0}^{\alpha_r},$$

where the operators M, W are given in (41) *and* (46) *respectively, $\alpha_j \geq 0$ for $0 \leq j \leq r$, and $l_{j'} \geq 1$ for $1 \leq j' \leq r$, and $r \geq 1$. Then for each integer $r \geq 0$,*

(i) $P_{\mathscr{H}} X_r\Big|_{\mathscr{H}} = Y_r$, *and*

(ii) $P_{\mathscr{F}\ominus\mathscr{H}} X_r\Big|_{\mathscr{F}\ominus\mathscr{H}} = P_{\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} X_r P_{\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})}\Big|_{\mathscr{F}\ominus\mathscr{H}}$.

Proof. Note that, it was obtained in the proof of [17, Theorem 2.3] that, for $r = 0, 1$,

$$P_{\mathscr{H}} X_r\Big|_{\mathscr{H}} = Y_r \tag{34}$$

For $r \geq 2$, to show $P_{\mathscr{H}} X_r\Big|_{\mathscr{H}} = Y_r$, we require the block matrix representations of M^n and V^n on the space $\mathscr{F} \oplus \mathcal{D}_T := \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathscr{H} \oplus \mathcal{D}_{T_0} \oplus S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \oplus \mathcal{D}_{T_1}$ for any $n \in \mathbb{N}$ and they are the following:

$$M^n = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & * \\ 0 & * & * & 0 & * \\ 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & * \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}, \tag{35}$$

and

$$\begin{aligned} V^n &= \begin{bmatrix} S^{*n}_{\mathcal{D}_{T_0^*}} & 0 & 0 \\ * & T_0^n & 0 \\ * & L_n & S^n_{\mathcal{D}_{T_0}} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \end{bmatrix} \\ &= \begin{bmatrix} S^{*n}_{\mathcal{D}_{T_0^*}} & 0 & 0 & 0 & 0 \\ * & T_0^n & 0 & 0 & 0 \\ * & D_{T_0} T_0^{n-1} & 0 & 0 & 0 \\ * & * & S^n_{\mathcal{D}_{T_0}} & S^n_{\mathcal{D}_{T_0}} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} : \\ &\quad \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \longrightarrow \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathscr{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}, \end{aligned} \tag{36}$$

where $*$ stands for some non-zero entries and $L_n = D_{T_0} T_0^{n-1} + S_{\mathcal{D}_{T_0}} L_{n-1}, L_0 = 0, n \geq 1$. Therefore using the structures (35) and (36) of M^n and V^n respectively

we conclude that

$$\begin{aligned}
&P_{\mathcal{H}}X_2\Big|_{\mathcal{H}}\\
&=P_{\mathcal{H}}V^{\alpha_0}P_{\mathcal{F}}((iM)^{l_1}V)V^{\alpha_1}P_{\mathcal{F}}((iM)^{l_2}V)V^{\alpha_2}\Big|_{\mathcal{H}}\\
&=P_{\mathcal{H}}V^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_1}P^{\perp}_{S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}V)V^{\alpha_1}\\
&\qquad\qquad\times P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_2}P^{\perp}_{S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}V)V^{\alpha_2}\Big|_{\mathcal{H}}\\
&=P_{\mathcal{H}}V^{\alpha_0}P_{\mathcal{H}}((iM)^{l_1}P^{\perp}_{S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}V)V^{\alpha_1}P_{\mathcal{H}}((iM)^{l_2}P^{\perp}_{S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}V)V^{\alpha_2}\Big|_{\mathcal{H}}\\
&=T_0^{\alpha_0}P_{\mathcal{H}}((iM)^{l_1}W)T_0^{\alpha_1}P_{\mathcal{H}}((iM)^{l_2}W)T_0^{\alpha_2}=Y_2,
\end{aligned}\tag{37}$$

and similarly for $r\geq 3$ we have

$$P_{\mathcal{H}}X_r\Big|_{\mathcal{H}}=T_0{}^{\alpha_0}P_{\mathcal{H}}\left((iM)^{l_1}W\right)T_0{}^{\alpha_1}\cdots P_{\mathcal{H}}\left((iM)^{l_r}W\right)T_0{}^{\alpha_r}=Y_r.\tag{38}$$

Note that for $r=0,1$, it was mentioned in the proof of [17, Theorem 2.3], that

$$P_{\mathcal{F}\ominus\mathcal{H}}X_r\Big|_{\mathcal{F}\ominus\mathcal{H}}=P_{\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}X_rP_{\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})}\Big|_{\mathcal{F}\ominus\mathcal{H}},$$

For $r\geq 2$, analyzing the structures of M^n and V^n as in (35) and (36) respectively we conclude that

$$\begin{aligned}
&P_{\mathcal{F}\ominus\mathcal{H}}X_r\Big|_{\mathcal{F}\ominus\mathcal{H}}\\
&=P_{\mathcal{F}\ominus\mathcal{H}}V^{\alpha_0}P_{\mathcal{F}}((iM)^{l_1}V)V^{\alpha_1}\cdots P_{\mathcal{F}}((iM)^{l_{r-1}}V)V^{\alpha_{r-1}}P_{\mathcal{F}}((iM)^{l_r}V)V^{\alpha_r}\Big|_{\mathcal{F}\ominus\mathcal{H}}\\
&=P_{\mathcal{F}\ominus\mathcal{H}}V^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}\\
&\qquad\cdots P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)\\
&\qquad\qquad\times V^{\alpha_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_r}\Big|_{\mathcal{F}\ominus\mathcal{H}}\\
&=P_{\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}V^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}\\
&\qquad\cdots P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}\\
&\qquad\qquad\times((iM)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_r}P_{\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})}\Big|_{\mathcal{F}\ominus\mathcal{H}}.
\end{aligned}\tag{39}$$

This completes the proof. □

Proof of Theorem 4.1. For $n=1,2$, property (32) and the formula (33) were established in [22, Section 2] and [17, Theorem 2.3]. Now we prove the theorem for $n\geq 3$. Following the steps of the proof of [17, Theorem 2.3], we first dilate T_0 to its minimal unitary dilation $V:=U_{T_0}$ on $\mathcal{F}=\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})\oplus\mathcal{H}\oplus\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})$, and then extend contraction T_1 to the contraction $T:=U_{T_1,T_0}$ on $\mathcal{F}=\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})\oplus\mathcal{H}\oplus\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})$. Now to apply our previous theorem, that is Theorem 3.2, we

dilate T to its minimal dilation $U_1 := U_T$ on $\mathcal{K} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus (\mathcal{F} \oplus \mathcal{D}_T) \oplus S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ and extend V to the unitary $U_0 := U_{V,T}$ on $\mathcal{K}$. Finally, following similar lines of argument of the proof of [17, Theorem 2.3], we conclude that there exists a self-adjoint operator $A \in \mathcal{B}_n(\mathcal{K})$ such that $U_1 = e^{iA}U_0$ with the block matrix representation

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{F} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{F} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}, \tag{40}$$

where

$$M = \begin{bmatrix} I & 0 & 0 & 0 & 0 \\ 0 & T_1T_0^* & T_1D_{T_0} & 0 & -D_{T_1^*}V_{T_1} \\ 0 & -V_{T_0}^*D_{T_0^*} & |T_0| & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & D_{T_1}T_0^* & D_{T_1}D_{T_0} & 0 & T_1^*V_{T_1} \end{bmatrix} \tag{41}$$

$$: \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}. \tag{42}$$

Therefore applying Theorem 3.2 corresponding to the pair (T, V) we conclude that for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\} \in \mathcal{B}_1(\mathcal{H}), \tag{43}$$

and there exists an $L^1([0, 2\pi])$-function ξ_n depend only on n, T and V such that

$$\mathrm{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it})\xi_n(t)dt, \tag{44}$$

where $V_s = P_{\mathcal{F}}e^{isM}V$, $s \in [0, 1]$. Our next aim is to show that for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\begin{aligned} &\mathrm{Tr}\left\{\phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(T_s)\right\} \\ =&\mathrm{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(V_s)\right\}, \end{aligned} \tag{45}$$

where

$$T_s = P_{\mathscr{H}} V_s\Big|_{\mathscr{H}} = P_{\mathscr{H}} e^{isB} \begin{bmatrix} 0 \\ T_0 \\ D_{T_0} \\ 0 \end{bmatrix} = P_{\mathscr{H}} e^{isM} W, \text{ where } W := V\Big|_{\mathscr{H}} = \begin{bmatrix} 0 \\ T_0 \\ D_{T_0} \\ 0 \end{bmatrix} \quad (46)$$

is a bounded operator from $\mathscr{H}$ to $\mathscr{F} \oplus \mathscr{D}_T$. Using Lemma 3.1 and Lemma 4.2 along with the similar type of arguments mentioned in the proof of Theorem 3.2, we conclude the identity (45). Thus the conclusion of the theorem follows by combining equations (44) and (45). This completes the proof.

□

5. Higher-order Trace formula for pair of maximal dissipative operators

In this section, our main aim is to prove the trace formula for pairs of maximal dissipative operators as an application of our main theorem in the previous section. We start with the section by recalling the definition of the dissipative operator. Let $A : \mathscr{H} \to \mathscr{H}$ be a linear operator (need not be bounded) with dense domain $\mathrm{Dom}(A)$ called dissipative if $\mathrm{Im}\langle Ah, h\rangle \leq 0$ for all $h \in \mathrm{Dom}(A)$. A dissipative operator is called maximal if it has no proper dissipative extension. It is well known that the Cayley transform of a maximal dissipative operator A is a contraction $T : \mathscr{H} \to \mathscr{H}$ given by $T = -(A+i)(A-i)^{-1}$ such that $\ker T = \ker(A+i)$ and $\ker T^* = \ker(A^* - i)$. Furthermore, if $\mathrm{Dom}(A) = \mathrm{Dom}(A^*)$, then the following pieces of information are also enlisted in [17], but for reader convenience and the self-containment of the article, we are providing it here as well with an appropriate modification of [17, Equation 2.11].

$$D_T = 2|(-\mathrm{Im}A)^{1/2}(A-i)^{-1}|, \quad D_{T^*} = 2|(-\mathrm{Im}A)^{1/2}(A^*+i)^{-1}|, \quad (47)$$

$$\mathscr{D}_T = \overline{((A^*+i)^{-1}(\mathrm{Im}A)\mathrm{Dom}(A))}, \quad \mathscr{D}_{T^*} = \overline{((A-i)^{-1}(\mathrm{Im}A)\mathrm{Dom}(A))}. \quad (48)$$

In the case of the dissipative operator we need a different class of functions different from the class considered in the last two sections. Let us consider the following class:

$$\mathcal{R}_n := \left\{\psi : \mathbb{R} \to \mathbb{C} \text{ such that } \psi(\lambda) = \phi\left(\frac{i+\lambda}{i-\lambda}\right) \text{ for some } \phi \in \mathcal{F}_n(\mathbb{T})\right\}.$$

Next we define $\psi_\pm$ using $\phi_\pm$ in a similar way as we have done in (8) and hence we obtain the decomposition $\psi(\lambda) = \psi_+(\lambda) + \psi_-(-\lambda)$. In other words, if $\psi \in \mathcal{R}_n$, then $\psi(\lambda) = \phi\left(\frac{i+\lambda}{i-\lambda}\right)$ for some $\phi \in \mathcal{F}_n(\mathbb{T})$, and

$$\psi_+(\lambda) = \phi_+\left(\frac{i+\lambda}{i-\lambda}\right) \text{ and } \psi_-(\lambda) = \phi_-\left(\frac{i+\lambda}{i-\lambda}\right).$$

Now we set

$$\psi_+(A) = \phi_+(T), \psi_+(-A^*) = \phi_-(T^*), \text{ and } \psi(A) = \psi_+(A) + \psi_-(-A^*).$$

The following lemma is essential to prove the main theorem in this section.

Lemma 5.1. *Let $\psi \in \mathcal{R}_n$ be such that $\psi(\lambda) = \phi\left(\frac{i+\lambda}{i-\lambda}\right)$ for some $\phi \in \mathcal{F}_n(\mathbb{T})$. Now if we substitute $z = e^{it} = \frac{i+\lambda}{i-\lambda}$, then $\phi(z) = \phi(e^{it}) = \psi(\lambda)$, $\lambda = -\tan\frac{t}{2}$, and for all $1 \le q \le n$,*

$$\phi^{(q)}(z) = \left(\sum_{k=0}^{q-1} p_{k,q}(\lambda)\, \psi^{(q-k)}(\lambda)\right)\frac{d\lambda}{dz}, \tag{49}$$

where $p_{k,q}$ are polynomials in λ of degree $(2(q-1)-k)$ and it is given recursively as follows

$p_{0,1}(\lambda) = 1$ *and for* $q \ge 2$

$$p_{k,q}(\lambda) = \begin{cases} (-i/2)(i-\lambda)^2\, p_{0,q-1}(\lambda) \\ \qquad\qquad \text{for } k = 0, \\ (-i/2)\left\{(i-\lambda)^2\left(p_{k,q-1}(\lambda) + p^{(1)}_{k-1,q-1}(\lambda)\right) + 2i(i-\lambda)p_{k-1,q-1}(\lambda)\right\} \\ \qquad\qquad \text{for } 1 \le k \le q-2, \\ (-i/2)\left[(i-\lambda)^2 p^{(1)}_{q-2,q-1}(\lambda) + 2i(i-\lambda)p_{q-2,q-1}(\lambda)\right] \\ \qquad\qquad \text{for } k = q-1. \end{cases}$$

Proof. We prove the identity (49) by the principle of mathematical induction. For $q = 1$, $\phi^{(1)}(z) = \psi^{(1)}(\lambda)\frac{d\lambda}{dz}$ and hence (49) is true for $q = 1$. Suppose (49) is true for $q = m \le n-1$, that is

$$\phi^{(m)}(z) = \left(\sum_{k=0}^{m-1} p_{k,m}(\lambda)\psi^{(m-k)}(\lambda)\right)\frac{d\lambda}{dz}.$$

Now we will show that (49) is also true for $q = m+1$. Note that

$$\begin{aligned} &\phi^{(m+1)}(z) \\ &= \sum_{k=0}^{m-1}\left[\left(p^{(1)}_{k,m}(\lambda)\psi^{(m-k)}(\lambda) + p_{k,m}(\lambda)\psi^{(m+1-k)}(\lambda)\right)\frac{d\lambda}{dz}\right. \\ &\quad \left. + (\lambda - i)p_{k,m}(\lambda)\psi^{(m-k)}(\lambda)\right]\frac{d\lambda}{dz} \\ &= p_{0,m}(\lambda)\psi^{(m+1)}(\lambda)\left(\frac{d\lambda}{dz}\right)^2 \\ &\quad + \sum_{k=0}^{m-2}\left[p_{k+1,m}(\lambda)\frac{d\lambda}{dz} + p^{(1)}_{k,m}(\lambda)\frac{d\lambda}{dz} + (\lambda - i)p_{k,m}(\lambda)\right]\psi^{(m-k)}(\lambda)\frac{d\lambda}{dz} \\ &\quad + \left[p^{(1)}_{m-1,m}(\lambda)\frac{d\lambda}{dz} + (\lambda - i)p_{m-1,m}(\lambda)\right]\psi^{(1)}(\lambda)\frac{d\lambda}{dz} \end{aligned}$$

$$
\begin{aligned}
&= p_{0,m}(\lambda)\psi^{(m+1)}(\lambda)\left(\frac{d\lambda}{dz}\right)^2 \\
&\quad + \sum_{k=1}^{m-1}\left[p_{k,m}(\lambda)\frac{d\lambda}{dz} + p^{(1)}_{k-1,m}(\lambda)\frac{d\lambda}{dz} + (\lambda - i)p_{k-1,m}(\lambda)\right] \\
&\quad \times \psi^{(m+1-k)}(\lambda)\frac{d\lambda}{dz} + \left[p^{(1)}_{m-1,m}(\lambda)\frac{d\lambda}{dz} + (\lambda - i)p_{m-1,m}(\lambda)\right]\psi^{(1)}(\lambda)\frac{d\lambda}{dz} \\
&= \left(\sum_{k=0}^{m} p_{k,m+1}(\lambda)\psi^{(m+1-k)}(\lambda)\right)\frac{d\lambda}{dz},
\end{aligned}
$$

where

$$
p_{k,m+1}(\lambda) = \begin{cases}
(-i/2)(i-\lambda)^2\, p_{0,m}(\lambda) & \\
\qquad\qquad \text{for } k = 0, & \\
(-i/2)\left\{(i-\lambda)^2\left(p_{k,m}(\lambda) + p^{(1)}_{k-1,m}(\lambda)\right) + 2i(i-\lambda)p_{k-1,m}(\lambda)\right\} & \\
\qquad\qquad \text{for } 1 \le k \le m-1, & \\
(-i/2)\left[(i-\lambda)^2 p^{(1)}_{m-1,m}(\lambda) + 2i(i-\lambda)p_{m-1,m}(\lambda)\right] & \\
\qquad\qquad \text{for } k = m, &
\end{cases}
$$

and degree of $p_{k,m+1}$ is $(2((m+1)-1)-k)$, and hence (49) is true for $q = m+1$. Therefore the result follows by the principle of mathematical induction. This completes the proof. □

Now we are in a position to state and prove our main result in this section. It is important to note that we make the hypothesis of our next theorem in such a way so that we can apply Theorem 4.1 to achieve our goal.

Theorem 5.2. *Let $n \in \mathbb{N}$. Let A_0 and A_1 be two maximal dissipative operators on $\mathscr{H}$ such that*

(*i*) $\dim\ker(A_j + i) = \dim\ker(A_j^* - i)$, *for* $j = 0, 1$,
(*ii*) $(A_1 - i)^{-1} - (A_0 - i)^{-1} \in \mathcal{B}_n(\mathscr{H})$, *and*
(*iii*) $\operatorname{Im} A_j = \dfrac{A_j - A_j^*}{2i} \in \mathcal{B}_{n/2}(\mathscr{H})$ *for* $j = 0, 1$.

Let $T_0 = -(A_0 + i)(A_0 - i)^{-1}$ and $T_1 = -(A_1 + i)(A_1 - i)^{-1}$ be the corresponding contractions obtained by the Cayley transform of maximal dissipative operators A_0 and A_1 respectively. Set $A_s = \left(i - 2i(T_s + 1)^{-1}\right)$, where T_s as in (31). *Then for $\psi \in \mathcal{R}_n$,*

$$
\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\psi(A_s)\right\} \in \mathcal{B}_1(\mathscr{H}),
$$

and there exists an $L^1([0,2\pi])$-function ξ_n depend only on n, A_1 and A_0 such that

$$\mathrm{Tr}\left\{\psi(A_1)-\psi(A_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\psi(A_s)\right\}=\int_0^{2\pi}\phi^{(n)}(e^{it})\xi_n(t)dt,$$

where $\psi(\lambda)=\phi\left(\frac{i+\lambda}{i-\lambda}\right)$ for some $\phi\in\mathcal{F}_n(\mathbb{T})$ and $\lambda\in\mathbb{R}$. Moreover, if $\psi\in\mathcal{S}(\mathbb{R})$ (Schwartz class of functions on $\mathbb{R}$), then there exists $\eta_n\in L^1\Big(\mathbb{R},(1+\lambda^2)^{-a}d\lambda\Big)$, $a>n$, such that

$$\mathrm{Tr}\left\{\psi(A_1)-\psi(A_0)-\sum_{k=0}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\psi(A_s)\right\}=\int_{-\infty}^{\infty}\psi^{(n)}(\lambda)\eta_n(\lambda)d\lambda.$$

Proof. Let $T_j=-(A_j+i)(A_j-i)^{-1}$ be the contraction obtained via the Cayley transform of a maximal dissipative operator A_j and hence $\ker T_j=\ker(A_j+i)$ and $\ker T_j^*=\ker(A_j^*-i)$ for $j=0,1$. Furthermore, note that

$$T_1-T_0=-2i\left[(A_1-i)^{-1}-(A_0-i)^{-1}\right].$$

Therefore using the hypothesis (i), (ii) and (iii) we conclude that the pair of contractions (T_0,T_1) on $\mathcal{H}$ satisfies the hypothesis (i) and (ii) of Theorem 4.1. Let V_j be the unitary operator on $\mathcal{H}$ such that $(A_j+i)(A_j-i)^{-1}=V_j|(A_j+i)(A_j-i)^{-1}|$ for $j=0,1$. Thus by applying Theorem 4.1 corresponding to the pair (T_0,T_1) we get for $\phi\in\mathcal{F}_n(\mathbb{T})$,

$$\left\{\phi(T_1)-\phi(T_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(T_s)\right\}\in\mathcal{B}_1(\mathcal{H}),\tag{50}$$

and there exists an $L^1([0,2\pi])$-function ξ_n depend only on n, T_1 and T_0 such that

$$\mathrm{Tr}\left\{\phi(T_1)-\phi(T_0)-\sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0}\phi(T_s)\right\}=\int_0^{2\pi}\phi^{(n)}(e^{it})\xi_n(t)dt,\tag{51}$$

where

$$T_s=P_{\mathcal{H}}e^{isM}\begin{bmatrix}0\\-(A_0+i)(A_0-i)^{-1}\\|2(-\mathrm{Im}A_0)^{1/2}(A_0-i)^{-1}|\\0\end{bmatrix},\ s\in[0,1],\tag{52}$$

and M is a self-adjoint operator on $\mathcal{F}\oplus\overline{\big((A_1^*+i)^{-1}(\mathrm{Im}A_1)\mathrm{Dom}(A_1)\big)}$ such that

$$\mathcal{F}=\mathbf{H}^2_{\overline{((A_0-i)^{-1}(\mathrm{Im}A_0)\mathrm{Dom}(A_0))}}(\mathbb{D})\oplus\mathcal{H}\oplus\mathbf{H}^2_{\overline{\big((A_0^*+i)^{-1}(\mathrm{Im}A_0)\mathrm{Dom}(A_0)\big)}}(\mathbb{D}),$$

$\sigma(M) \subseteq (-\pi, \pi]$, $M \in \mathcal{B}_n(\mathcal{F} \oplus \overline{\left((A_1^* + i)^{-1}(\mathrm{Im}A_1)\mathrm{Dom}(A_1)\right)})$ (the block matrix representation of e^{iM} is same as the block matrix representation of H mentioned in the proof of [17, Theorem 2.5]).

Now it easy to observe that for $\psi(\lambda) = \phi\left(\frac{i+\lambda}{i-\lambda}\right) \in \mathcal{R}_n$, where $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\begin{aligned}&\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\\ &= \phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s), \end{aligned} \tag{53}$$

where $A_s = \left(i - 2i(T_s + 1)^{-1}\right)$. Therefore using equations (50), (51) and (53) we conclude that

$$\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1([0, 2\pi])$-function ξ_n depend only on n, A_1 and A_0 such that

$$\mathrm{Tr}\left\{\psi(A_1) - \psi(A_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it}) \xi_n(t) dt,$$

which by applying Lemma 5.1 yields that

$$\begin{aligned}&\mathrm{Tr}\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\}\\ &= \int_{-\infty}^{\infty} \left(\sum_{k=0}^{n-1} p_{k,n}(\lambda) \psi^{(n-k)}(\lambda)\right) \zeta_n(\lambda) d\lambda, \end{aligned} \tag{54}$$

where $\zeta_n(\lambda) = i(\lambda - i)(i + \lambda)^{-1} \xi_n(-2tan^{-1}(\lambda))$ and $\zeta_n \in L^1\left(\mathbb{R}, (1 + \lambda^2)^{-1} d\lambda\right)$. In particular, if we consider $\psi \in \mathcal{S}(\mathbb{R}) \subset \mathcal{R}_n$, then by performing integration by-parts (54) becomes

$$\mathrm{Tr}\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\} = \int_{-\infty}^{\infty} \psi^{(n)}(\lambda) \eta_n(\lambda) d\lambda,$$

where

$$\eta_n(\lambda) = \left[\sum_{k=0}^{n-1} (-1)^k \eta_{k,k}^n(\lambda)\right], \ \eta_{0,0}^n(\lambda) = p_{0,n}(\lambda) \zeta_n(\lambda),$$

$$\eta^n_{1,1}(\lambda) = \int_0^\lambda p_{1,n}(\mu)\zeta_n(\mu)\,d\mu, \text{ and for } k \geq 2,$$

$$\eta^n_{j,k}(\lambda) = \begin{cases} \int_0^\lambda p_{k,n}(\mu)\,\zeta_n(\mu)\,d\mu & \text{if } j = 1, \\ \int_0^\lambda \eta^n_{j-1,k}(\mu)\,d\mu & \text{if } 2 \leq j \leq k. \end{cases}$$

This completes the proof. □

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