

Sun's Series via Cyclotomic Multiple Zeta Values

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Abstract. We prove and generalize several recent conjectures of Z.-W. Sun surrounding binomial coefficients and harmonic numbers. We show that Sun's series and their analogs can be represented as cyclotomic multiple zeta values of levels $N \in \{4, 8, 12, 16, 24\}$, namely Goncharov's multiple polylogarithms evaluated at N -th roots of unity.

Key words: Sun's series; binomial coefficients; harmonic numbers; cyclotomic multiple zeta values

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1 Introduction

Amongst Zhi-Wei Sun's recent conjectures [19, Section 2] concerning binomial coefficients $\binom{m}{k} := \frac{m!}{k!(m-k)!}$ for $m \in \mathbb{Z}_{\geq 0}$, $k \in \mathbb{Z} \cap [0, m]$ and harmonic numbers $H_m^{(r)} := \sum_{k=1}^m \frac{1}{k^r}$ of order $r \in \mathbb{Z}_{>0}$ for $m \in \mathbb{Z}_{\geq 0}$, one can find certain (\mathbb{Q} -linear combinations of) convergent series in the following type:

$$\sum_{k=1}^{\infty} \frac{\binom{2k}{k}^n}{k^s} \left(\frac{t}{2^{2n}}\right)^k \left[\prod_{j=1}^M H_{k-1}^{(r_j)} \right] \left[\prod_{j'=1}^{M'} H_{2k-1}^{(r'_{j'})} \right], \quad (1.1)$$

where $n \in \{-1, 1\}$, $s \in \mathbb{Z}$, $M, M' \in \mathbb{Z}_{\geq 0}$, and $|t| < 1$. Such infinite series were previously known as “inverse binomial sums” and “binomial sums” in some literature of high energy physics [1, 3, 9, 10, 15, 16, 20] that revolved around a certain class of Feynman diagrams. If one allows $n = 0$ in (1.1), then one recovers some special cases of the “nested harmonic sums” studied by mathematical physicists [4, 5].

In our recent work [23, Section 3], we have analyzed (1.1) for $n \in \{-1, 0, 1\}$, effectively reaching the following conclusion: if t is an algebraic number satisfying $|t| < 1$, then the infinite sum in (1.1) can be represented as a $\mathbb{Q}(\pi)$ -linear combination of Goncharov's multiple polylogarithms (MPLs) [12, 13]

$$\text{Li}_{a_1, \dots, a_n}(z_1, \dots, z_n) := \sum_{\ell_1 > \dots > \ell_n > 0} \prod_{j=1}^n \frac{z_j^{\ell_j}}{\ell_j^{a_j}}, \quad (1.2)$$

where $a_1, \dots, a_n \in \mathbb{Z}_{>0}$ are positive integers and $z_1, \dots, z_n \in \overline{\mathbb{Q}}$ are explicitly computable algebraic numbers. For meticulously chosen algebraic numbers $t \in \overline{\mathbb{Q}}$, we can sometimes confine the arguments z_1, \dots, z_n of our MPLs to roots of unity, arriving at members of

$$\mathfrak{Z}_k(N) := \text{span}_{\mathbb{Q}} \left\{ \text{Li}_{a_1, \dots, a_n}(z_1, \dots, z_n) \in \mathbb{C} \mid \right. \\ \left. a_1, \dots, a_n \in \mathbb{Z}_{>0}, z_1^N = \dots = z_n^N = 1, \sum_{j=1}^n a_j = k \right\}, \quad (1.3)$$

the \mathbb{Q} -vector space spanned by cyclotomic multiple zeta values (CMZVs) of weight $k \in \mathbb{Z}_{>0}$ and level $N \in \mathbb{Z}_{>0}$. In [23, Section 3], we have achieved our aforementioned goals by converting (1.1) into certain $\overline{\mathbb{Q}}(\pi)$ -linear combinations of contour integrals

$$\int_C \text{Li}_{a_1, \dots, a_n}(z_1(t), \dots, z_n(t)) \frac{dt}{R(t)} \quad (1.4)$$

for $z_1(t), \dots, z_n(t), R(t) \in \overline{\mathbb{Q}}(t)$, and evaluating these integrals via fibrations of MPLs [18, Lemma 2.14 and Corollary 3.2]. Originating from the seminal works of Davydychev–Kalmykov [9, 10], the integral formulation (1.4) of the infinite series in (1.1) was followed up by Weinzierl [20], Ablinger [1, 2], Au [6, 7], and Xu–Zhao [21, 22] among other researchers, prior to our study in [23, Section 3].

Special values of MPLs at algebraic arguments already cover a wide class of mathematical constants, such as $\log 2 = \text{Li}_1(\frac{1}{2}) = -\text{Li}_1(-1)$, $G = \frac{1}{2i} [\text{Li}_2(i) - \text{Li}_2(-i)]$, and $\zeta(3) = \text{Li}_3(1)$. Furthermore, the versatility of MPLs allows us to compute sophisticated series whose exact values are hard to discover empirically. For instance, from [23, Table 7] one may read off¹

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(2k+1)^3} \frac{(-1)^k}{2^{4k}} = \frac{25 \text{Re Li}_3(e^{2\pi i/5})}{12} + \frac{\zeta(3)}{2} \in \mathfrak{Z}_3(5), \\ \sum_{k=0}^{\infty} \frac{\binom{2k}{k} \text{H}_{2k+1}}{(2k+1)^2} \frac{(-1)^k}{2^{4k}} = -5 \text{Re Li}_3(e^{2\pi i/5}) + \frac{8\zeta(3)}{5} \in \mathfrak{Z}_3(5),$$

which combine into an identity

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k} (5\text{H}_{2k+1} + \frac{12}{2k+1})}{(2k+1)^2 (-16)^k} = 14\zeta(3)$$

found by Sun and proved by Charlton–Gangl–Lai–Xu–Zhao [8, Section 4].

In Section 2 of this note, we extrapolate [23, Corollary 3.8] to the theorem below.

Theorem 1.1 (Sun’s series involving $\binom{2k}{k}$ and harmonic numbers). *For $r \in \mathbb{Z}_{>1}$, we have the following CMZV characterizations:*

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} \text{H}_k^{(r)} = \oint_{|z|=1} \frac{\text{Li}_r\left(\frac{(1+z)^2}{8z}\right)}{1 - \frac{(1+z)^2}{8z}} \frac{dz}{2\pi iz} \in \sqrt{2}\mathfrak{Z}_r(8), \quad (1.5)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} \text{H}_{2k}^{(r)} = \oint_{|z|=1} \left[\frac{\text{Li}_r\left(\frac{1+z^2}{2\sqrt{2}z}\right)}{1 - \frac{1+z^2}{2\sqrt{2}z}} + \frac{\text{Li}_r\left(-\frac{1+z^2}{2\sqrt{2}z}\right)}{1 + \frac{1+z^2}{2\sqrt{2}z}} \right] \frac{dz}{4\pi iz} \in \sqrt{2}\mathfrak{Z}_r(8), \quad (1.6)$$

¹In what follows, we abbreviate $\text{H}_m^{(1)}$ into H_m .

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_k^{(r)} = \oint_{|z|=1} \frac{\operatorname{Li}_r\left(\frac{(1+z)^2}{16z}\right)}{1 - \frac{(1+z)^2}{16z}} \frac{dz}{2\pi iz} \in \sqrt{3}\mathfrak{Z}_r(12), \quad (1.7)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_{2k}^{(r)} = \oint_{|z|=1} \left[\frac{\operatorname{Li}_r\left(\frac{1+z^2}{4z}\right)}{1 - \frac{1+z^2}{4z}} + \frac{\operatorname{Li}_r\left(-\frac{1+z^2}{4z}\right)}{1 + \frac{1+z^2}{4z}} \right] \frac{dz}{4\pi iz} \in \sqrt{3}\mathfrak{Z}_r(12). \quad (1.8)$$

Remark 1.2. For $r = 2$ (resp. $r = 3$), one may reorganize the formulas below into series involving $H_{2k}^{(r)} - \frac{1}{2^r} H_k^{(r)}$ in [19, Theorem 1.1] (resp. [19, Conjectures 2.2 and 2.3]):

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} H_k^{(2)} &= -12\sqrt{2} \operatorname{Li}_2(\sqrt{2}-1) - 4\sqrt{2}\tilde{\lambda}^2 + \frac{11\pi^2}{6\sqrt{2}} \in \sqrt{2}\mathfrak{Z}_2(8), \\ \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} H_k^{(3)} &= -\frac{128\sqrt{2}}{3} \operatorname{Re} \operatorname{Li}_3(e^{\pi i/4}) + 72\sqrt{2} \operatorname{Li}_3\left(\frac{1}{\sqrt{2}}\right) - 48\sqrt{2} \operatorname{Li}_3(\sqrt{2}-1) \\ &\quad - \frac{39\zeta(3)}{4\sqrt{2}} + 12\sqrt{2}(3\lambda - 2\tilde{\lambda}) \operatorname{Li}_2(\sqrt{2}-1) \\ &\quad + \frac{9(\pi^2 - \lambda^2)\lambda - [12\tilde{\lambda}(2\tilde{\lambda} - 9\lambda) + 54\lambda^2 + 11\pi^2]\tilde{\lambda}}{3\sqrt{2}} \in \sqrt{2}\mathfrak{Z}_3(8), \end{aligned}$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} H_{2k}^{(2)} &= \frac{\pi^2}{16\sqrt{2}} + \frac{1}{4} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} H_k^{(2)} \in \sqrt{2}\mathfrak{Z}_2(8), \\ \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} H_{2k}^{(3)} &= \frac{35\sqrt{2}\zeta(3)}{64} - \frac{\sqrt{2}\pi G}{8} + \frac{1}{8} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k} H_k^{(3)} \in \sqrt{2}\mathfrak{Z}_3(8), \\ \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_k^{(2)} &= -\frac{32 \operatorname{Li}_2(2-\sqrt{3})}{\sqrt{3}} - \frac{4\tilde{\Lambda}^2}{\sqrt{3}} + \frac{5\pi^2}{3\sqrt{3}} \in \sqrt{3}\mathfrak{Z}_2(12), \\ \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_k^{(3)} &= -\frac{288}{\sqrt{3}} \operatorname{Re} \operatorname{Li}_3(e^{\pi i/6}) - \frac{256 \operatorname{Li}_3(2-\sqrt{3})}{\sqrt{3}} - \frac{64}{\sqrt{3}} \operatorname{Li}_3\left(1 - \frac{\sqrt{3}}{2}\right) \\ &\quad + \frac{256}{\sqrt{3}} \operatorname{Li}_3\left(\frac{\sqrt{3}-1}{2}\right) + 76\sqrt{3}\zeta(3) + \frac{64(2\lambda - \tilde{\Lambda}) \operatorname{Li}_2(2-\sqrt{3})}{\sqrt{3}} \\ &\quad + \frac{2[24(\tilde{\Lambda} - \lambda)\lambda\tilde{\Lambda} - 5\pi^2\tilde{\Lambda} + 8\lambda^3]}{3\sqrt{3}} \in \sqrt{3}\mathfrak{Z}_3(12), \end{aligned}$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_{2k}^{(2)} &= \frac{\pi^2}{36\sqrt{3}} + \frac{1}{4} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_k^{(2)} \in \sqrt{3}\mathfrak{Z}_2(12), \\ \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_{2k}^{(3)} &= \frac{2\zeta(3)}{3\sqrt{3}} - \frac{\pi \operatorname{Im} \operatorname{Li}_2(e^{2\pi i/3})}{4\sqrt{3}} + \frac{1}{8} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{16^k} H_k^{(3)} \in \sqrt{3}\mathfrak{Z}_3(12), \end{aligned}$$

where

$$\lambda := \log 2, \quad \tilde{\lambda} := \log(1 + \sqrt{2}), \quad \tilde{\Lambda} := \log(2 + \sqrt{3}).$$

In Section 3, we adapt our recent work [23, Corollary 3.8] to scenarios involving the binomial coefficients $\binom{3k}{k}$ and $\binom{4k}{2k}$, thereby accommodating to some of Sun's new conjectures [19, Section 2] announced on June 5, 2023. Our results are summarized in the next two theorems.

Theorem 1.3 (CMZVs in Sun's series involving $\binom{3k}{k}$, $\binom{4k}{2k}$ and harmonic numbers).

(a) We have

$$\sum_{k=1}^{\infty} \frac{1}{k^s 2^k \binom{3k}{k}} = \begin{cases} \int_0^1 \frac{\frac{t(1-t)^2}{2}}{1 - \frac{t(1-t)^2}{2}} \frac{dt}{t} = \frac{\pi}{10} - \frac{\log 2}{5}, & s = 1, \\ \int_0^1 \text{Li}_{s-1} \left(\frac{t(1-t)^2}{2} \right) \frac{dt}{t} \in \mathfrak{Z}_s(4), & s \in \mathbb{Z}_{>1}, \end{cases} \quad (1.9)$$

$$\sum_{k=1}^{\infty} \frac{H_{3k} - H_k + \frac{1}{k}}{k^s 2^k \binom{3k}{k}} = \begin{cases} - \int_0^1 \frac{\frac{t(1-t)^2}{2} \log t}{1 - \frac{t(1-t)^2}{2}} dt = \frac{2G}{5} - \frac{\log^2 2}{10}, & s = 1, \\ - \int_0^1 \text{Li}_{s-1} \left(\frac{t(1-t)^2}{2} \right) \log t \frac{dt}{t} \in \mathfrak{Z}_{s+1}(4), & s \in \mathbb{Z}_{>1}, \end{cases} \quad (1.10)$$

$$\sum_{k=1}^{\infty} \frac{H_{3k} - H_{2k}}{k^s 2^k \binom{3k}{k}} = \begin{cases} - \int_0^1 \frac{\frac{t(1-t)^2}{2} \log(1-t)}{1 - \frac{t(1-t)^2}{2}} \frac{dt}{t} \\ = \frac{2G}{5} + \frac{\log^2 2}{10} - \frac{\pi \log 2}{20} - \frac{\pi^2}{40}, & s = 1, \\ - \int_0^1 \text{Li}_{s-1} \left(\frac{t(1-t)^2}{2} \right) \log(1-t) \frac{dt}{t} \in \mathfrak{Z}_{s+1}(4), & s \in \mathbb{Z}_{>1}. \end{cases} \quad (1.11)$$

(b) For $r \in \mathbb{Z}_{>0}$, the following formulas hold true:

$$\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_k^{(r)} = \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \frac{\text{Li}_r \left(\frac{2X^3}{(1+X^3)^2} \right)}{1 - \frac{2X^3}{(1+X^3)^2}} \frac{dX}{1+X^3} \in \mathfrak{Z}_r(12) + \sqrt{3}\mathfrak{Z}_r(12), \quad (1.12)$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_{2k}^{(r)} &= \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \left[\frac{\text{Li}_r \left(\frac{\sqrt{2}x^3}{1+x^6} \right)}{1 - \frac{\sqrt{2}x^3}{1+x^6}} + \frac{\text{Li}_r \left(-\frac{\sqrt{2}x^3}{1+x^6} \right)}{1 + \frac{\sqrt{2}x^3}{1+x^6}} \right] \frac{x dx}{1+x^6} \\ &\in \mathfrak{Z}_r(24) + \sqrt{3}\mathfrak{Z}_r(24), \end{aligned} \quad (1.13)$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} (3H_{3k} - 2H_{2k} - H_k - 3 \log 3) H_k^{(r)} \\ = \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \frac{\text{Li}_r \left(\frac{2X^3}{(1+X^3)^2} \right) \log \frac{X^3}{(1+X^3)^2}}{1 - \frac{2X^3}{(1+X^3)^2}} \frac{dX}{1+X^3} \in \mathfrak{Z}_{r+1}(12) + \sqrt{3}\mathfrak{Z}_{r+1}(12). \end{aligned} \quad (1.14)$$

In addition, one has

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} (3H_{3k} - 2H_{2k} - H_k - 3 \log 3) &= \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \frac{\log \frac{X^3}{(1+X^3)^2}}{1 - \frac{2X^3}{(1+X^3)^2}} \frac{dX}{1+X^3} \\ &= -\frac{3 + \sqrt{3}}{2} \log 2 - \sqrt{3} \log(2 + \sqrt{3}) \in \mathfrak{Z}_1(12) + \sqrt{3}\mathfrak{Z}_1(12). \end{aligned} \quad (1.15)$$

(c) For $r \in \mathbb{Z}_{>0}$, we have

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{4k}{2k}}{2^{5k}} H_k^{(r)} &= \frac{2\sqrt{2}}{\pi} \int_0^{\infty} \frac{\text{Li}_r \left(\frac{2X^4}{(1+X^4)^2} \right)}{1 - \frac{2X^4}{(1+X^4)^2}} \frac{X^2 dX}{1+X^4} \\ &\in \sqrt{1 + \frac{1}{\sqrt{2}}} \mathfrak{Z}_r(16) + \sqrt{1 - \frac{1}{\sqrt{2}}} \mathfrak{Z}_r(16), \end{aligned} \quad (1.16)$$

$$\sum_{k=0}^{\infty} \frac{3^k \binom{4k}{2k}}{2^{6k}} H_k^{(r)} = \frac{2\sqrt{2}}{\pi} \int_0^{\infty} \frac{\text{Li}_r\left(\frac{3X^4}{(1+X^4)^2}\right) X^2 dX}{1 - \frac{3X^4}{(1+X^4)^2}} \in \mathfrak{Z}_r(24) + \sqrt{3}\mathfrak{Z}_r(24). \quad (1.17)$$

Remark 1.4. Part (a) of the theorem above uses ideas from Kam Cheong Au (see [6, Example 4.21] and [7, Proposition 7.13]). Some formulas below were previously reported by Au, while the rest prove and generalize Sun's experimental identities [19, formulas (2.6) and (2.7) in Conjecture 2.4]:

$$\begin{aligned} \sum_{k=1}^{\infty} \frac{1}{k^2 2^k \binom{3k}{k}} &= \frac{\pi^2}{24} - \frac{\lambda^2}{2} \in \mathfrak{Z}_2(2) \subset \mathfrak{Z}_2(4), \\ \sum_{k=1}^{\infty} \frac{1}{k^3 2^k \binom{3k}{k}} &= -\frac{33\zeta(3)}{16} + \pi G + \frac{\lambda^3}{6} - \frac{\pi^2 \lambda}{24} \in \mathfrak{Z}_3(4), \\ \sum_{k=1}^{\infty} \frac{1}{k^4 2^k \binom{3k}{k}} &= -\frac{21}{2} \text{Li}_4\left(\frac{1}{2}\right) + 2\pi \text{Im Li}_3\left(\frac{1+i}{2}\right) \\ &\quad - \frac{57\zeta(3)\lambda}{8} - \frac{23\lambda^4}{48} + \frac{19\pi^2 \lambda^2}{48} + \frac{61\pi^4}{960} \in \mathfrak{Z}_4(4), \\ \sum_{k=1}^{\infty} \frac{H_{3k} - H_k}{k^2 2^k \binom{3k}{k}} &= \frac{2G}{5} + \frac{2\lambda^2}{5} - \frac{\pi^2}{24} \in \mathfrak{Z}_2(2) + i\mathfrak{Z}_2(4), \\ \sum_{k=1}^{\infty} \frac{H_{3k} - H_k}{k^2 2^k \binom{3k}{k}} &= \frac{11\zeta(3)}{4} - \pi G - \frac{\pi^2 \lambda}{24} \in \mathfrak{Z}_3(4), \\ \sum_{k=1}^{\infty} \frac{H_{3k} - H_k}{k^3 2^k \binom{3k}{k}} &= \frac{27}{2} \text{Li}_4\left(\frac{1}{2}\right) - 2\pi \text{Im Li}_3\left(\frac{1+i}{2}\right) \\ &\quad + \frac{145\zeta(3)\lambda}{16} + 2G^2 + \frac{9\lambda^4}{16} - \frac{23\pi^2 \lambda^2}{48} - \frac{17\pi^4}{160} \in \mathfrak{Z}_4(4), \\ \sum_{k=1}^{\infty} \frac{H_{2k} - H_k}{k^2 2^k \binom{3k}{k}} &= \frac{3\lambda^2}{10} + \frac{\pi\lambda}{20} - \frac{\pi^2}{60} \in \mathfrak{Z}_2(2) + i\mathfrak{Z}_2(4), \\ \sum_{k=1}^{\infty} \frac{H_{2k} - H_k}{k^2 2^k \binom{3k}{k}} &= \frac{33\zeta(3)}{32} - \frac{\pi G}{2} + \frac{\pi^2 \lambda}{24} \in \mathfrak{Z}_3(4), \\ \sum_{k=1}^{\infty} \frac{H_{2k} - H_k}{k^3 2^k \binom{3k}{k}} &= \frac{9}{2} \text{Li}_4\left(\frac{1}{2}\right) + \frac{93\zeta(3)\lambda}{32} + \frac{\pi G \lambda}{2} + \frac{3\lambda^4}{16} - \frac{5\pi^2 \lambda^2}{24} - \frac{31\pi^4}{640} \in \mathfrak{Z}_4(4), \end{aligned}$$

where $\lambda := \log 2$ and $G := \text{Im Li}_2(i)$.

It is possible to extend the statements in part (a) to $s \in \mathbb{Z}_{\leq 0}$, but the resulting patterns are not as neat as the $s \in \mathbb{Z}_{>1}$ cases. For example, we have

$$\begin{aligned} \sum_{k=1}^{\infty} \frac{H_{3k} - 8H_{2k} + 7H_k}{2^k \binom{3k}{k}} &= \int_0^1 x \frac{d}{dx} \frac{x}{1-x} \Big|_{x=\frac{t(1-t)^2}{2}} \frac{\log \frac{t^7}{(1-t)^8}}{t} dt + 7 \int_0^1 \frac{\frac{t(1-t)^2}{2}}{1 - \frac{t(1-t)^2}{2}} \frac{dt}{t} \\ &= \frac{22G}{125} - \frac{2 \log^2 2}{25} - \frac{22\pi \log 2}{125} - \frac{17\pi^2}{1500} - \frac{33 \log 2}{25} + \frac{11\pi}{50} \end{aligned}$$

and

$$\sum_{k=1}^{\infty} \frac{H_{3k} - 8H_{2k} + 7H_k}{2^k \binom{3k}{k}} k = \int_0^1 \left(x \frac{d}{dx} \right)^2 \frac{x}{1-x} \Big|_{x=\frac{t(1-t)^2}{2}} \frac{\log \frac{t^7}{(1-t)^8}}{t} dt$$

$$\begin{aligned}
& + 7 \int_0^1 x \frac{d}{dx} \frac{x}{1-x} \Big|_{x=\frac{t(1-t)^2}{2}} \frac{dt}{t} \\
& = \frac{316G}{3125} - \frac{6 \log^2 2}{625} - \frac{316\pi \log 2}{3125} - \frac{17\pi^2}{12500} - \frac{549 \log 2}{625} + \frac{33\pi}{1250}.
\end{aligned}$$

These two equations conjoin into a succinct formula

$$\sum_{k=1}^{\infty} \frac{H_{3k} - 8H_{2k} + 7H_k}{2^k \binom{3k}{k}} (25k - 3) = 2G - 2(\pi + 9) \log 2$$

that has been discovered recently by Sun [19, formula (2.10) in Conjecture 2.5].

Remark 1.5. Part (b) of the theorem above and its accompanying formulas below verify and extend Sun's recent observations [19, formulas (2.12)–(2.13) in Conjecture 2.6]:

$$\begin{aligned}
\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_k &= \frac{3 - \sqrt{3}}{2} \lambda - \frac{3(\sqrt{3} + 1)}{4} \Lambda + \sqrt{3} \tilde{\Lambda} \in \mathfrak{Z}_1(12) + \sqrt{3} \mathfrak{Z}_1(12), \\
\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_k^{(2)} &= -12\sqrt{3} \operatorname{Li}_2 \left(\frac{\sqrt{3} - 1}{2} \right) + 3(\sqrt{3} - 1) \operatorname{Li}_2(2 - \sqrt{3}) + \frac{3(\sqrt{3} - 1)}{2} \operatorname{Li}_2 \left(\frac{1}{4} \right) \\
&\quad + \frac{3[(2\sqrt{3} - 3)\lambda^2 - 2(2\sqrt{3} - 1)\lambda\tilde{\Lambda} - \tilde{\Lambda}^2]}{4} + \frac{(7\sqrt{3} + 3)\pi^2}{12} \\
&\in \mathfrak{Z}_2(12) + \sqrt{3} \mathfrak{Z}_2(12), \\
\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_{2k} &= \frac{3 - \sqrt{3}}{4} \lambda - \frac{3(\sqrt{3} + 1)}{4} (\Lambda - \tilde{\Lambda}) \in \mathfrak{Z}_1(12) + \sqrt{3} \mathfrak{Z}_1(12) \\
&\subset \mathfrak{Z}_1(24) + \sqrt{3} \mathfrak{Z}_1(24), \\
\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} \tilde{h}_k &= -\frac{3 + \sqrt{3}}{2} \lambda - \sqrt{3} \tilde{\Lambda} \in \mathfrak{Z}_1(12) + \sqrt{3} \mathfrak{Z}_1(12), \\
\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} \tilde{h}_k H_k &= -30\sqrt{3} \operatorname{Li}_2 \left(\frac{\sqrt{3} - 1}{2} \right) + 3(\sqrt{3} - 1) \operatorname{Li}_2(2 - \sqrt{3}) + \frac{15}{4} (\sqrt{3} - 1) \operatorname{Li}_2 \left(\frac{1}{4} \right) \\
&\quad + \frac{6(1 - 5\sqrt{3})\lambda\tilde{\Lambda} + 6\sqrt{3}\Lambda\tilde{\Lambda} - 3(3\sqrt{3} + 1)\tilde{\Lambda}^2 + (17\sqrt{3} - 33)\lambda^2}{4} \\
&\quad + \frac{3(\sqrt{3} + 3)\lambda\Lambda}{4} + \frac{(13\sqrt{3} + 3)\pi^2}{8} \in \mathfrak{Z}_2(12) + \sqrt{3} \mathfrak{Z}_2(12),
\end{aligned}$$

where $\lambda := \log 2$, $\Lambda := \log 3$, $\tilde{\Lambda} := \log(2 + \sqrt{3})$, and $\tilde{h}_k := 3H_{3k} - 2H_{2k} - H_k - 3 \log 3$.

Remark 1.6. In part (c) of the theorem above, we do not need dedicated spaces for convergent series like (cf. [19, Remark 2.8])

$$\sum_{k=0}^{\infty} \binom{4k}{2k} z^{2k} H_{2k}^{(r)} = \frac{1}{2} \sum_{k=0}^{\infty} \binom{2k}{k} [z^k + (-z)^k] H_k^{(r)}, \tag{1.18}$$

$$\sum_{k=0}^{\infty} \binom{4k}{2k} z^{2k} H_{4k}^{(r)} = \frac{1}{2} \sum_{k=0}^{\infty} \binom{2k}{k} [z^k + (-z)^k] H_{2k}^{(r)}, \tag{1.19}$$

since the right-hand sides of these two equations are fully characterized by [19, formulas (1.1) and (1.2)] for $r = 1$, and by (2.5')–(2.6') in Section 2.2 below for $r \in \mathbb{Z}_{>1}$.

Theorem 1.7 (logarithms in Sun's series involving $\binom{3k}{k}$, $\binom{4k}{2k}$ and harmonic numbers).

(a) If $\varphi \in (0, \pi/3)$, then we have

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left(4 \cos^2 \frac{3\varphi}{2}\right)^k \mathbf{H}_k &= \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \frac{\operatorname{Li}_1\left(\frac{4X^3 \cos^2 \frac{3\varphi}{2}}{(1+X^3)^2}\right)}{1 - \frac{4X^3 \cos^2 \frac{3\varphi}{2}}{(1+X^3)^2}} \frac{dX}{1+X^3} \\ &= \frac{\sqrt{3}}{\sin \frac{3\varphi}{2}} \left[\cos \frac{\varphi}{2} \log \frac{2 \cos^2 \left(\frac{\varphi}{2} - \frac{\pi}{3}\right)}{\sqrt{3} \sin \varphi} + \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right) \log \frac{2 \cos^2 \frac{\varphi}{2}}{\sqrt{3} \sin \left(\frac{2\pi}{3} - \varphi\right)} \right], \end{aligned} \quad (1.20)$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left(4 \cos^2 \frac{3\varphi}{2}\right)^k (3\mathbf{H}_{3k} - 2\mathbf{H}_{2k} - \mathbf{H}_k - 3 \log 3) \\ &= \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \frac{\log \frac{X^3}{(1+X^3)^2}}{1 - \frac{4X^3 \cos^2 \frac{3\varphi}{2}}{(1+X^3)^2}} \frac{dX}{1+X^3} \\ &= -\frac{2\sqrt{3}}{\sin \frac{3\varphi}{2}} \left[\cos \frac{\varphi}{2} \log \left(2 \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right)\right) + \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right) \log \left(2 \cos \frac{\varphi}{2}\right) \right], \end{aligned} \quad (1.21)$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left(2 \cos \frac{3\varphi}{2}\right)^{2k} \mathbf{H}_{2k} \\ &= \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \left[\frac{\operatorname{Li}_1\left(\frac{2x^3 \cos \frac{3\varphi}{2}}{1+x^6}\right)}{1 - \frac{2x^3 \cos \frac{3\varphi}{2}}{1+x^6}} + \frac{\operatorname{Li}_1\left(-\frac{2x^3 \cos \frac{3\varphi}{2}}{1+x^6}\right)}{1 + \frac{2x^3 \cos \frac{3\varphi}{2}}{1+x^6}} \right] \frac{x dx}{1+x^6} = \frac{\sqrt{3}}{\sin \frac{3\varphi}{2}} \\ &\times \left[\cos \frac{\varphi}{2} \log \frac{2 \cos \frac{\varphi}{2} \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right)}{\sqrt{3} \sin \varphi} + \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right) \log \frac{2 \cos \frac{\varphi}{2} \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right)}{\sqrt{3} \sin \left(\frac{2\pi}{3} - \varphi\right)} \right]. \end{aligned} \quad (1.22)$$

(b) If $\psi \in (0, \pi/4)$, then we have

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{4k}{2k}}{2^{6k}} (4 \cos^2 2\psi)^k \mathbf{H}_k \\ &= \frac{2\sqrt{2}}{\pi} \int_0^{\infty} \frac{\operatorname{Li}_1\left(\frac{4X^4 \cos^2 2\psi}{(1+X^4)^2}\right)}{1 - \frac{4X^4 \cos^2 2\psi}{(1+X^4)^2}} \frac{X^2 dX}{1+X^4} = \frac{\log \frac{(\csc \psi + \sqrt{2})^2}{4(\cot \psi + 1)}}{\sqrt{2} \sin \psi} + \frac{\log \frac{(\sec \psi + \sqrt{2})^2}{4(\tan \psi + 1)}}{\sqrt{2} \cos \psi}. \end{aligned} \quad (1.23)$$

Remark 1.8. Picking $\varphi = \pi/6$ in part (a) of the theorem above, we recover some entries of Remark 1.5. Plugging $\varphi = 2\pi/15$ into

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left(4 \cos^2 \frac{3\varphi}{2}\right)^k (\mathbf{H}_{3k} - \mathbf{H}_{2k}) = \frac{\cos \frac{\varphi}{2} + \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right)}{\sqrt{3} \sin \frac{3\varphi}{2}} \log \frac{3}{4 \cos \frac{\varphi}{2} \cos \left(\frac{\varphi}{2} - \frac{\pi}{3}\right)},$$

we arrive at

$$\sum_{k=0}^{\infty} \binom{3k}{k} \left(\frac{3 + \sqrt{5}}{54}\right)^k (\mathbf{H}_{3k} - \mathbf{H}_{2k}) = \frac{1 + \sqrt{5}}{2} \left(\log 3 - 2 \log \frac{1 + \sqrt{5}}{2} \right),$$

as suggested by Sun [19, formula (2.15) in Conjecture 2.7].

Remark 1.9. Together with the right-hand sides of (1.18)–(1.19) for $r = 1$, part (b) of the theorem above answers a question of Sun [19, formula (2.16) in Conjecture 2.8].

Remark 1.10. For $\psi \in \{\pi/8, \pi/12\}$, one can paraphrase (1.23) as

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{4k}{2k}}{2^{5k}} H_k &= \sqrt{1 + \frac{1}{\sqrt{2}}} \operatorname{Re} \left[7 \operatorname{Li}_1(e^{\pi i/8}) + 7 \operatorname{Li}_1(e^{3\pi i/8}) + 7 \operatorname{Li}_1(e^{5\pi i/8}) + 3 \operatorname{Li}_1(e^{7\pi i/8}) \right] \\ &\quad + \sqrt{1 - \frac{1}{\sqrt{2}}} \operatorname{Re} \left[\operatorname{Li}_1(e^{\pi i/8}) - 3 \operatorname{Li}_1(e^{3\pi i/8}) + \operatorname{Li}_1(e^{5\pi i/8}) + \operatorname{Li}_1(e^{7\pi i/8}) \right], \\ \sum_{k=0}^{\infty} \frac{3^k \binom{4k}{2k}}{2^{6k}} H_k &= 2 \operatorname{Re} [\operatorname{Li}_1(e^{\pi i/6}) + \operatorname{Li}_1(e^{2\pi i/3})] + 2\sqrt{3} \operatorname{Re} [2 \operatorname{Li}_1(e^{\pi i/6}) + 3 \operatorname{Li}_1(e^{\pi i/2})], \end{aligned}$$

thus testifying to (1.16) and (1.17).

2 CMZV characterizations of certain series involving $\binom{2k}{k}$

2.1 Recursions and fibrations of polylogarithms

Adopting the notational conventions of Frellesvig–Tommasini–Wever [11, Section 2], we define Goncharov’s generalized polylogarithm (GPL) recursively by an integral along a straight line segment

$$G(\alpha_1, \dots, \alpha_n; z) := \int_0^z \frac{G(\alpha_2, \dots, \alpha_n; x) dx}{x - \alpha_1} \quad (2.1)$$

for $|\alpha_1|^2 + \dots + |\alpha_n|^2 \neq 0$, with the extra settings that

$$G(\underbrace{0, \dots, 0}_m; z) := \frac{\log^m z}{m!}, \quad G(-; z) := 1. \quad (2.2)$$

These GPLs are related to MPLs [defined in (1.2)] by the following equation (see [18, formula (1.3)] or [11, formula (2.6)])

$$G\left(\underbrace{0, \dots, 0}_{a_1-1}, \tilde{\alpha}_1, \underbrace{0, \dots, 0}_{a_2-1}, \tilde{\alpha}_2, \dots, \underbrace{0, \dots, 0}_{a_n-1}, \tilde{\alpha}_n; z\right) = (-1)^n \operatorname{Li}_{a_1, \dots, a_n} \left(\frac{z}{\tilde{\alpha}_1}, \frac{\tilde{\alpha}_1}{\tilde{\alpha}_2}, \dots, \frac{\tilde{\alpha}_{n-1}}{\tilde{\alpha}_n} \right) \quad (2.3)$$

when $\prod_{j=1}^n \tilde{\alpha}_j \neq 0$. As a result of this GPL-MPL correspondence, we may reformulate (1.3) as

$$\mathfrak{Z}_k(N) := \operatorname{span}_{\mathbb{Q}} \{ G(z_1, \dots, z_k; 1) \mid z_1^N, \dots, z_k^N \in \{0, 1\}, z_1 \neq 1, z_k \neq 0 \}. \quad (1.3')$$

Here, the convergence of $G(z_1, \dots, z_k; 1)$ requires that $z_1 \neq 1$, while (2.3) stipulates that $z_k \neq 0$.

Echoing the GPL recursion (2.1) for a special class of MPLs

$$\operatorname{Li}_k(z) = -G(\underbrace{0, \dots, 0}_{k-1}, 1; z),$$

we analytically continue polylogarithms $\operatorname{Li}_k(z) := \sum_{n=1}^{\infty} \frac{z^k}{n^k}$, $|z| < 1$ [cf. (1.2)] to all $z \in \mathbb{C} \setminus [1, \infty)$, by

$$\begin{aligned} \operatorname{Re} \operatorname{Li}_1(z) &:= -\log |1 - z|, \\ \operatorname{Im} \operatorname{Li}_1(z) &:= -\arg(1 - z) \in [-\pi, \pi), \\ \operatorname{Li}_{k+1}(z) &:= \int_0^z \operatorname{Li}_k(w) \frac{dw}{w}, \quad k \in \mathbb{Z}_{>0}, \end{aligned}$$

where the integration path is also a straight line segment. With the recursive definition of polylogarithms, one can show inductively that

$$\operatorname{Li}_k(x + i0^+) - \operatorname{Li}_k(x - i0^+) = \frac{2\pi i}{(k-1)!} \log^{k-1} x \quad (2.4)$$

holds for all $x \in (1, \infty)$ and $k \in \mathbb{Z}_{>0}$.

In the rest of this note, we will frequently need to integrate the differential 1-form

$$G(\alpha_1(t), \dots, \alpha_n(t); z(t)) \frac{dt}{R(t)}$$

over certain contours, where $\alpha_1(t), \dots, \alpha_n(t)$, $z(t)$, $R(t)$ are rational functions of t . To fully exploit the recursion (2.1) while evaluating such contour integrals, we take fibration procedures [18, Lemma 2.14 and Corollary 3.2] to rewrite $G(\alpha_1(t), \dots, \alpha_n(t); z(t))$ in terms of finitely many new GPLs in the shape of $G(\beta_1, \dots, \beta_n; t)$, where the constants β_1, \dots, β_n are sorted from the zeros and poles of the rational functions $z(t) - \alpha_j(t)$, $\alpha_j(t) - \alpha_{j'}(t)$, $\alpha_n(t)$ for $j, j' \in \mathbb{Z} \cap [1, n]$.

For example, the branch cut analysis in [23, Corollary 3.8 (a)] brings us the following fibration structure for $r \in \mathbb{Z}_{>1}$ and $4|\chi| \leq |1 + \chi|^2$:

$$\begin{aligned} \oint_{|z|=1} \frac{\operatorname{Li}_r\left(\frac{\chi(1+z)^2}{z(1+\chi)^2}\right) dz}{1 - \frac{\chi(1+z)^2}{z(1+\chi)^2}} \frac{1}{2\pi i z} &= \frac{1+\chi}{1-\chi} \oint_{|z|=1} \left(\frac{1}{z-\chi} - \frac{1}{z-\frac{1}{\chi}} \right) \operatorname{Li}_r\left(\frac{\chi(1+z)^2}{z(1+\chi)^2}\right) \frac{dz}{2\pi i} \\ &\in \frac{1+\chi}{1-\chi} \operatorname{span}_{\mathbb{Q}} \{(\pi i)^{r-\ell} G(\alpha_1, \dots, \alpha_\ell; \chi) \in \mathbb{C} \mid \alpha_1^2, \dots, \alpha_\ell^2 \in \{0, 1\}, \ell \in \mathbb{Z} \cap [0, r]\} \\ &=: \frac{1+\chi}{1-\chi} \mathfrak{H}_r^{(\chi)}(2), \end{aligned} \quad (2.5)$$

while the argument in [23, Corollary 3.8 (b)] leads us to the following relation for $r \in \mathbb{Z}_{>1}$ and $2|v| \leq |1 + v^2|$:

$$\begin{aligned} \oint_{|z|=1} \frac{\operatorname{Li}_r\left(\pm \frac{v(1+z^2)}{z(1+v^2)}\right) dz}{1 \mp \frac{v(1+z^2)}{z(1+v^2)}} \frac{1}{2\pi i z} &= \frac{1+v^2}{1-v^2} \oint_{|z|=1} \left(\frac{1}{z \mp v} - \frac{1}{z \mp \frac{1}{v}} \right) \operatorname{Li}_r\left(\pm \frac{v(1+z^2)}{z(1+v^2)}\right) \frac{dz}{2\pi i} \\ &\in \frac{1+v^2}{1-v^2} \operatorname{span}_{\mathbb{Q}} \{(\pi i)^{r-\ell} G(\alpha_1, \dots, \alpha_\ell; v) \in \mathbb{C} \mid \alpha_1^4, \dots, \alpha_\ell^4 \in \{0, 1\}, \ell \in \mathbb{Z} \cap [0, r]\} \\ &=: \frac{1+v^2}{1-v^2} \mathfrak{H}_r^{(v)}(4). \end{aligned} \quad (2.6)$$

Here in both (2.5) and (2.6), the integrands are pole-free when the contours are shrunk to tight loops wrapping around the branch cuts of polylogarithms, because the jump discontinuities in (2.4) tend to zero as $x \rightarrow 1 + 0^+$, for $k \in \mathbb{Z}_{>1}$.

2.2 Some CMZVs of levels 8 and 12

With the foregoing preparations, we are ready for the verification of our claims in (1.5)–(1.8).

Proof of Theorem 1.1. Recall that [17, Section 5.1]

$$\sum_{k=1}^{\infty} w^k \mathbf{H}_k^{(r)} = \frac{\operatorname{Li}_r(w)}{1-w} \quad (2.7)$$

holds for $|w| < 1$, $r \in \mathbb{Z}_{>0}$, and

$$\oint_{|z|=1} \left[\frac{(1+z)^2}{z} \right]^k \frac{dz}{2\pi iz} = \frac{1}{2\pi} \int_0^{2\pi} \left(4 \cos^2 \frac{\theta}{2} \right)^k d\theta = \binom{2k}{k}.$$

Thus, for $4|\chi| \leq |1 + \chi|^2$, the relation

$$\sum_{k=0}^{\infty} \binom{2k}{k} \left[\frac{\chi}{(1+\chi)^2} \right]^k \mathbf{H}_k^{(r)} = \oint_{|z|=1} \frac{\text{Li}_r \left(\frac{\chi(1+z)^2}{z(1+\chi)^2} \right)}{1 - \frac{\chi(1+z)^2}{z(1+\chi)^2}} \frac{dz}{2\pi iz} \in \frac{1+\chi}{1-\chi} \mathfrak{H}_r^{(\chi)}(2) \quad (2.5')$$

is immediate from termwise integration and reference to (2.5). Likewise, from

$$\sum_{k=1}^{\infty} w^{2k} \mathbf{H}_{2k}^{(r)} = \frac{\text{Li}_r(w)}{1-w} + \frac{\text{Li}_r(-w)}{1+w} \quad (2.8)$$

for $|w| < 1$, $r \in \mathbb{Z}_{>0}$, one deduces the following relation for $2|v| \leq |1 + v^2|$:

$$\begin{aligned} \sum_{k=0}^{\infty} \binom{2k}{k} \left(\frac{v}{1+v^2} \right)^{2n} \mathbf{H}_{2k}^{(r)} &= \oint_{|z|=1} \left[\frac{\text{Li}_r \left(\frac{v(1+z^2)}{z(1+v^2)} \right)}{1 - \frac{v(1+z^2)}{z(1+v^2)}} + \frac{\text{Li}_r \left(-\frac{v(1+z^2)}{z(1+v^2)} \right)}{1 + \frac{v(1+z^2)}{z(1+v^2)}} \right] \frac{dz}{2\pi iz} \\ &\in \frac{1+v^2}{1-v^2} \mathfrak{H}_r^{(v)}(4), \end{aligned} \quad (2.6')$$

upon referring to (2.6). Thus, with specially chosen parameters

$$\frac{\chi}{(1+\chi)^2} = \begin{cases} \frac{1}{8}, & \chi = (\sqrt{2}-1)^2, \\ \frac{1}{16}, & \chi = (2-\sqrt{3})^2, \end{cases} \quad \left(\frac{v}{1+v^2} \right)^2 = \begin{cases} \frac{1}{8}, & v = \sqrt{2}-1, \\ \frac{1}{16}, & v = 2-\sqrt{3}, \end{cases}$$

we have confirmed the equalities in (1.5)–(1.8).

To build the remaining halves of (1.5)–(1.8) on the knowledge of (2.5') and (2.6'), we notice that

$$\frac{1+\chi}{1-\chi} = \begin{cases} \frac{\sqrt{2}}{2}, & \chi = (\sqrt{2}-1)^2, \\ \frac{2}{\sqrt{3}}, & \chi = (2-\sqrt{3})^2, \end{cases} \quad \frac{1+v^2}{1-v^2} = \begin{cases} \frac{\sqrt{2}}{2}, & v = \sqrt{2}-1, \\ \frac{2}{\sqrt{3}}, & v = 2-\sqrt{3}, \end{cases}$$

while the `IterIntDoableQ` function in Au's `MultipleZetaValues` package (v1.2.0) [7] certifies that

$$\mathfrak{H}_r^{(\chi)}(2) \subset \begin{cases} \mathfrak{Z}_r(8), & \chi = (\sqrt{2}-1)^2, \\ \mathfrak{Z}_r(12), & \chi = (2-\sqrt{3})^2, \end{cases} \quad \mathfrak{H}_r^{(v)}(4) \subset \begin{cases} \mathfrak{Z}_r(8), & v = \sqrt{2}-1, \\ \mathfrak{Z}_r(12), & v = 2-\sqrt{3}. \end{cases}$$

Au's abovementioned package produces analytic evaluations of integrals like (1.5)–(1.8), so long as the results are in the \mathbb{Q} -vector spaces $\mathfrak{Z}_k(8)$, $k \in \{1, 2, 3, 4\}$ or $\mathfrak{Z}_k(12)$, $k \in \{1, 2, 3\}$, hence Remark 1.2. \blacksquare

In the proof above and some arguments in the next section, we are effectively dealing with special cases of Au's integrals [7, Section 3]

$$\int_a^b R_0(x) \text{Li}_{r_1}(R_1(x)) \cdots \text{Li}_{r_k}(R_k(x)) dx, \quad (2.9)$$

where the 1-form $R_0(x)dx$ has only simple poles on the complex sphere, and the functions $R_j(x)$, $1 \leq j \leq k$, are rational. One may find out the structure of (2.9) by looking at a finite set S that is the union of $\{a, b, \infty\}$ with $R_j^{-1}(0)$, $R_j^{-1}(1)$, $R_j^{-1}(\infty)$ for $1 \leq j \leq k$ and all the poles of $R_0(x)dx$. If S is a subset of $\{0, \infty\} \cup \{e^{2\pi im/N} | m \in \mathbb{Z} \cap [1, N]\}$, then (2.9) is expressible through CMZVs of level N . In some other situations, feeding the set $S \setminus \{\infty\}$ to the `IterIntDoableQ` function in Au's `MultipleZetaValues` package (v1.2.0) [7], one may also receive a CMZV level $N \leq 12$ that is compatible with our analysis. However, residue calculus is still required in order to obtain the correct $\overline{\mathbb{Q}}$ -linear combinations of CMZVs in Theorems 1.1, 1.3, and 1.7, and to eliminate extraneous factors of $\frac{1}{2\pi i}$.

3 CMZV and logarithmic characterizations of certain series involving $\binom{3k}{k}$ and $\binom{4k}{2k}$

3.1 Integral representations of $\binom{3k}{k}^{\pm 1}$ and $\binom{4k}{2k}$

It is an elementary exercise in Euler's (di)gamma functions that

$$\begin{aligned} \frac{1}{k \binom{3k}{k}} &= \int_0^1 [t(1-t)^2]^k \frac{dt}{t}, \\ \frac{H_{3k} - H_k + \frac{1}{k}}{k \binom{3k}{k}} &= - \int_0^1 [t(1-t)^2]^k \log t \frac{dt}{t}, \\ \frac{H_{3k} - H_{2k}}{k \binom{3k}{k}} &= - \int_0^1 [t(1-t)^2]^k \log(1-t) \frac{dt}{t}. \end{aligned}$$

These identities support the integral representations of infinite series in (1.9)–(1.11), in conjunction with the generating function (2.7) for harmonic numbers.

One can verify

$$\frac{2\pi}{3\sqrt{3}} \frac{\binom{3k}{k}}{3^{3k}} = \int_0^\infty \left[\frac{X^3}{(1+X^3)^2} \right]^k \frac{dX}{1+X^3} \quad (3.1)$$

and its equivalent form (up to a variable substitution $X = x^2$)

$$\frac{\pi}{3\sqrt{3}} \frac{\binom{3k}{k}}{3^{3k}} = \int_0^\infty \left(\frac{x^3}{1+x^6} \right)^{2k} \frac{x dx}{1+x^6} \quad (3.1')$$

by manipulating an integral representation for Euler's beta function [14, item 8.380.3]. The derivative of (3.1) with respect to k leaves us

$$\frac{2\pi}{3\sqrt{3}} \frac{\binom{3k}{k}}{3^{3k}} (3H_{3k} - 2H_{2k} - H_k - 3 \log 3) = \int_0^\infty \left[\frac{X^3}{(1+X^3)^2} \right]^k \frac{\log \frac{X^3}{(1+X^3)^2} dX}{1+X^3}. \quad (3.2)$$

Therefore, the generating function (2.7) brings us the equalities between series and integrals in (1.12)–(1.15) and (1.20)–(1.22). In fact, as long as the inequalities $|1 + \Xi^3|^2 < 4|\Xi^3|$ and $|1 + \xi^6| < 2|\xi^3|$ are honored, we have the following extensions (cf. (2.7), (2.8), (3.1), (3.1'), and (3.2)) of (1.20)–(1.22):

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left[\frac{(1 + \Xi^3)^2}{\Xi^3} \right]^k H_k^{(r)} = \frac{3\sqrt{3}}{2\pi} \int_0^\infty \frac{\text{Li}_r \left(\frac{X^3(1+\Xi^3)^2}{\Xi^3(1+X^3)^2} \right)}{1 - \frac{X^3(1+\Xi^3)^2}{\Xi^3(1+X^3)^2}} \frac{dX}{1+X^3},$$

$$\begin{aligned}
& \sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left[\frac{(1+\Xi^3)^2}{\Xi^3} \right]^k (3H_{3k} - 2H_{2k} - H_k - 3 \log 3) H_k^{(r)} \\
&= \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \frac{\text{Li}_r \left(\frac{X^3(1+\Xi^3)^2}{\Xi^3(1+X^3)^2} \right) \log \frac{X^3}{(1+X^3)^2} dX}{1 - \frac{X^3(1+\Xi^3)^2}{\Xi^3(1+X^3)^2}} \frac{1}{1+X^3}, \\
& \sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \left(\frac{1+\xi^6}{\xi^3} \right)^{2k} H_{2k}^{(r)} = \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} \left[\frac{\text{Li}_r \left(\frac{x^3(1+\xi^6)}{\xi^3(1+x^6)} \right)}{1 - \frac{x^3(1+\xi^6)}{\xi^3(1+x^6)}} + \frac{\text{Li}_r \left(-\frac{x^3(1+\xi^6)}{\xi^3(1+x^6)} \right)}{1 + \frac{x^3(1+\xi^6)}{\xi^3(1+x^6)}} \right] \frac{x dx}{1+x^6}
\end{aligned}$$

for $r \in \mathbb{Z}_{>0}$.

Akin to (3.1), we have

$$\frac{\pi}{2\sqrt{2}} \frac{\binom{4k}{2k}}{2^{6k}} = \int_0^{\infty} \left[\frac{X^4}{(1+X^4)^2} \right]^k \frac{X^2 dX}{1+X^4},$$

so termwise integration of the generating function (2.7) steers us to

$$\sum_{k=0}^{\infty} \frac{\binom{4k}{2k}}{2^{6k}} \left[\frac{(1+\Xi^4)^2}{\Xi^4} \right]^k H_k^{(r)} = \frac{2\sqrt{2}}{\pi} \int_0^{\infty} \frac{\text{Li}_r \left(\frac{X^4(1+\Xi^4)^2}{\Xi^4(1+X^4)^2} \right) X^2 dX}{1 - \frac{X^4(1+\Xi^4)^2}{\Xi^4(1+X^4)^2}} \frac{1}{1+X^4}$$

for $|1+\Xi^4|^2 < 4|\Xi^4|$ and $r \in \mathbb{Z}_{>0}$, which proves *a fortiori* the equalities in (1.16)–(1.17) and (1.23).

3.2 Some CMZVs of levels 4, 12, 16, and 24

We start by treating the CMZVs of level 4 appearing in (1.9)–(1.11).

Proof of Theorem 1.3 (a). First we demonstrate the following fibration structure for $r \in \mathbb{Z}_{>0}$:

$$\text{Li}_r \left(\frac{t(1-t)^2}{2} \right) \in \text{span}_{\mathbb{Z}} \{ G(\beta_1, \dots, \beta_r; t) \mid \beta_j \in \{0, 1\}, j \in \mathbb{Z} \cap [1, r); \beta_r \in \{2, i, -i\} \}. \quad (3.3)$$

Clearly, the claim is true for

$$\text{Li}_1 \left(\frac{t(1-t)^2}{2} \right) = -G(2; t) - G(i; t) - G(-i; t).$$

From

$$\text{Li}_r \left(\frac{t(1-t)^2}{2} \right) = \int_0^t \left(\frac{1}{s} + \frac{2}{s-1} \right) \text{Li}_{r-1} \left(\frac{s(1-s)^2}{2} \right) ds$$

and the GPL recursion (2.1), we may verify (3.3) inductively.

Appealing again to the GPL recursion (2.1), we see that

$$\begin{aligned}
& \int_0^1 \text{Li}_r \left(\frac{t(1-t)^2}{2} \right) \frac{dt}{t} \\
& \in \text{span}_{\mathbb{Z}} \{ G(0, \beta_1, \dots, \beta_r; 1) \mid \beta_j \in \{0, 1\}, j \in \mathbb{Z} \cap [1, r); \beta_r \in \{2, i, -i\} \}.
\end{aligned}$$

Here, it is evident from the definition of $\mathfrak{Z}_k(N)$ in (1.3') that

$$\text{span}_{\mathbb{Z}} \{ G(0, \beta_1, \dots, \beta_r; 1) \mid \beta_j \in \{0, 1\}, j \in \mathbb{Z} \cap [1, r); \beta_r \in \{i, -i\} \} \subset \mathfrak{Z}_{r+1}(4).$$

Meanwhile, either a variable substitution in (2.1) or a special case of the Hölder relation [11, formula (2.13)] leads us to $G(0, \beta_1, \dots, \beta_{r-1}, 2; 1) = (-1)^{r+1} G(-1, 1 - \beta_{r-1}, \dots, 1 - \beta_1, 1; 1)$, so it follows that

$$\text{span}_{\mathbb{Z}}\{G(0, \beta_1, \dots, \beta_{r-1}, 2; 1) \mid \beta_j \in \{0, 1\}, j \in \mathbb{Z} \cap [1, r]\} \subset \mathfrak{Z}_{r+1}(2) \subseteq \mathfrak{Z}_{r+1}(4).$$

This completes the verification of (1.9).

Before extending such a service to (1.10) and (1.11), we note that the shuffle product of GPLs [11, formula (2.4)] implies

$$\begin{aligned} G(\alpha; t)G(\beta_1, \dots, \beta_r; t) &= G(\alpha, \beta_1, \dots, \beta_r; t) + \sum_{j=1}^{r-1} G(\beta_1, \dots, \beta_j, \alpha, \beta_{j+1}, \dots, \beta_r; t) \\ &\quad + G(\beta_1, \dots, \beta_r, \alpha; t), \end{aligned} \quad (3.4)$$

and especially

$$\begin{aligned} 0 &= G(0; 1)G(\beta_1, \dots, \beta_r; 1) = G(0, \beta_1, \dots, \beta_r; 1) + \sum_{j=1}^{r-1} G(\beta_1, \dots, \beta_j, 0, \beta_{j+1}, \dots, \beta_r; 1) \\ &\quad + G(\beta_1, \dots, \beta_r, 0; 1) \end{aligned} \quad (3.4')$$

for $G(0; 1) = \log 1 = 0$ [cf. (2.2)]. In other words, an extra factor of $\log t = G(0; t)$ or $\log(1-t) = G(1; t)$ in the integrand of (1.10) or (1.11) modifies the fibration structure on the right-hand side of (3.3) into $\beta_1, \dots, \beta_{r+1} \in \{0, 1, i, -i\}$ or $\beta_1, \dots, \beta_{r+1} \in \{0, 1, 2\}$, and $\beta_{r+1} \neq 0$. This accounts for the CMZV characterizations in (1.10) and (1.11). ■

As we have just seen, the fibration structure of GPLs plays pivotal rôles in the CMZV characterization at level $N = 4$. The same will apply to the $N \in \{12, 24\}$ situations at the next stage.

For technical reasons related to the branch cuts of polylogarithms [see (2.4)], we will focus on the $\mathfrak{Z}_k(N)$, $k \in \mathbb{Z}_{>1}$ cases in this subsection, deferring the treatment of $\mathfrak{Z}_1(N)$ to Section 3.3.

Proof of Theorem 1.3 (b) for $\mathfrak{Z}_k(12)$ and $\mathfrak{Z}_k(24)$, where $k \in \mathbb{Z}_{>1}$. Begin with an equivalent formulation of the equality in (1.12):

$$\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_k^{(r)} = \frac{3\sqrt{3}}{2\pi} \frac{1}{1 - e^{2\pi i/3}} \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^{\infty} \right) \frac{\text{Li}_r \left(\frac{2X^3}{(1+X^3)^2} \right)}{1 - \frac{2X^3}{(1+X^3)^2}} \frac{dX}{1 + X^3}, \quad (1.12')$$

where the contour consists of two rays passing through the origin in the complex X -plane, whose angles of inclination are 120° and 0° respectively. Had we traded X for $1/X$ in (1.12) before such a conversion, we would have ended up with

$$\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_k^{(r)} = \frac{3\sqrt{3}}{2\pi} \frac{1}{1 - e^{4\pi i/3}} \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^{\infty} \right) \frac{\text{Li}_r \left(\frac{2X^3}{(1+X^3)^2} \right)}{1 - \frac{2X^3}{(1+X^3)^2}} \frac{X dX}{1 + X^3} \quad (1.12'')$$

instead. Averaging over (1.12') and (1.12''), we arrive at

$$\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} H_k^{(r)} = \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^{\infty} \right) \text{Li}_r \left(\frac{2z^3}{(1+z^3)^2} \right) R_{12}(z) \frac{dz}{2\pi i}, \quad (1.12^*)$$

where the rational function

$$R_{12}(z) := \frac{3\sqrt{3}i}{2} \left(\frac{1}{1 - e^{2\pi i/3}} + \frac{z}{1 - e^{4\pi i/3}} \right) \frac{1}{1 - \frac{2z^3}{(1+z^3)^2}} \frac{1}{1 + z^3}$$

has only six simple poles located at $e^{(2m-1)\pi i/6}$, $m \in \mathbb{Z} \cap [1, 6]$, with all the corresponding residues being in the \mathbb{Q} -vector space $\mathbb{Q} + \mathbb{Q}\sqrt{3}$. Thanks to Cauchy's integral formula, we obtain

$$\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} \mathbf{H}_k^{(r)} = \lim_{\varepsilon \rightarrow 0^+} \int_{C_\varepsilon^{[\pi/6, \pi/2]}} \text{Li}_r \left(\frac{2z^3}{(1+z^3)^2} \right) R_{12}(z) \frac{dz}{2\pi i}, \quad (1.12^{**})$$

where the counterclockwise contour $C_\varepsilon^{[\alpha, \beta]}$ is separated from the circular arc $e^{i\theta}$, $\theta \in [\alpha, \beta]$ by a distance ε . In other words, we will need to focus on the branch cut discontinuities of the integrand in (1.12**), which satisfy [cf. (2.4) and (3.4)]

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0^+} \left[\text{Li}_r \left(\frac{2[(1+\varepsilon)e^{i\theta}]^3}{\{1 + [(1+\varepsilon)e^{i\theta}]^3\}^2} \right) - \text{Li}_r \left(\frac{2[(1-\varepsilon)e^{i\theta}]^3}{\{1 + [(1-\varepsilon)e^{i\theta}]^3\}^2} \right) \right] \\ &= \pi i \frac{\theta - \frac{\pi}{3}}{\left| \theta - \frac{\pi}{3} \right|} \frac{\log^{r-1} \frac{2e^{3i\theta}}{(1+e^{3i\theta})^2}}{(r-1)!} \\ &\in 2\pi i \frac{\theta - \frac{\pi}{3}}{\left| \theta - \frac{\pi}{3} \right|} \text{span}_{\mathbb{Q}} \{ G(\beta_1, \dots, \beta_{r-1-\ell}; e^{i\theta}) \log^\ell 2 \mid \\ & \quad \beta_j^3 \in \{0, -1\}, j \in \mathbb{Z} \cap [1, r-1-\ell]; \ell \in \mathbb{Z} \cap [0, r-1] \} \end{aligned}$$

for $\theta \in [\pi/6, \pi/3) \cup (\pi/3, \pi/2]$. Bearing in mind the filtration property $\mathfrak{Z}_j(N)\mathfrak{Z}_k(N) \subseteq \mathfrak{Z}_{j+k}(N)$ for $j, k \in \mathbb{Z}_{\geq 0}$ [13, Section 1.2], along with the fact that $\log 2 = -\text{Li}_1(-1) \in \mathfrak{Z}_1(2) \subset \mathfrak{Z}_1(12)$, we may turn (1.12**) into

$$\begin{aligned} & \sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} \mathbf{H}_k^{(r)} \in \text{span}_{\mathbb{Q}} \left\{ \lim_{\varepsilon \rightarrow 0^+} \left[\int_{(1-\varepsilon)e^{\pi i/6}}^{(1-\varepsilon)e^{\pi i/2}} - \int_{(1+\varepsilon)e^{\pi i/6}}^{(1+\varepsilon)e^{\pi i/2}} \right] R_{12}(z) \right. \\ & \quad \times \left. \frac{\arg z - \frac{\pi}{3}}{\left| \arg z - \frac{\pi}{3} \right|} G(\beta_1, \dots, \beta_{r-1-\ell}; z) \log^\ell 2 dz \mid \right. \\ & \quad \left. \beta_j^{12} \in \{0, 1\}, j \in \mathbb{Z} \cap [1, r-1-\ell]; \ell \in \mathbb{Z} \cap [0, r-1] \right\} \\ & \subseteq \text{span}_{\mathbb{Q} + \mathbb{Q}\sqrt{3}} \{ G(\beta_1, \dots, \beta_{r-\ell}; z) \log^\ell 2 \mid \\ & \quad z^{12} = 1; \beta_j^{12} \in \{0, 1\}, j \in \mathbb{Z} \cap [1, r-\ell]; \ell \in \mathbb{Z} \cap [0, r-1] \} \subseteq \mathfrak{Z}_r(12) + \sqrt{3}\mathfrak{Z}_r(12) \end{aligned}$$

upon integrating over the branch cut discontinuities across a circular arc, via Panzer's logarithmic regularizations [18, Section 2.3] that cancel out $O(\log^r \varepsilon)$ contributions from individual GPL recursions (2.1). Here, before arriving at the set inclusion in the last step, we have used the scaling property [11, formula (2.3)] of GPLs $G(\mu\alpha_1, \dots, \mu\alpha_n; \mu z) = G(\alpha_1, \dots, \alpha_n; z)$ for $\mu \neq 0$, $\alpha_n \neq 0$, the shuffle algebra of GPLs (see (3.4) and (3.4') above), as well as the relation $\pi i \in \mathfrak{Z}_1(N)$ for $N \in \mathbb{Z}_{\geq 3}$ [7, Lemma 4.1], to confirm that

$$\mathfrak{Z}_k(N) = \text{span}_{\mathbb{Q}} \{ G(z_1, \dots, z_k; z) \mid z_1^N, \dots, z_k^N \in \{0, 1\}, z^N = 1, z_1 \neq z \} \quad (1.3'')$$

for $N \in \mathbb{Z}_{\geq 3}$. So far, we have verified (1.12) in its entirety.

To prove (1.14), we need to deform the contour in

$$\sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} (3\mathbf{H}_{3k} - 2\mathbf{H}_{2k} - \mathbf{H}_k + \log 2 - 3 \log 3) \mathbf{H}_k^{(r)}$$

$$= \left(\int_0^{\infty} + \int_{\infty e^{2\pi i/3}}^0 \right) \left[\text{Li}_r \left(\frac{2z^3}{(1+z^3)^2} \right) \log \frac{2z^3}{(1+z^3)^2} \right] R_{12}(z) \frac{dz}{2\pi i}. \quad (1.14^*)$$

Like (2.5) and (2.6), the integrand in (1.14*) is pole-free when the new contour wraps around the branch cuts tightly. In addition to an integral over the loop $C_\varepsilon^{[\pi/6, \pi/2]}$ as in the last paragraph, we also need to take into account the jump discontinuities attributed to the factor $\log \frac{2z^3}{(1+z^3)^2}$, which are located at a ray running from 0 to $\infty e^{\pi i/3}$. Exploiting the symmetry of the integral under a reflection $z \mapsto e^{2\pi i/3}/z$, we can check that

$$\begin{aligned} & \left(\int_{\delta e^{\pi i/3-i0^+}}^{\frac{1}{\delta} e^{\pi i/3-i0^+}} - \int_{\delta e^{\pi i/3+i0^+}}^{\frac{1}{\delta} e^{\pi i/3+i0^+}} \right) \left[\text{Li}_r \left(\frac{2z^3}{(1+z^3)^2} \right) \log \frac{2z^3}{(1+z^3)^2} \right] R_{12}(z) \frac{dz}{2\pi i} \\ &= 2 \left(\int_{\delta e^{\pi i/3-i0^+}}^{e^{\pi i/3-i0^+}} - \int_{\delta e^{\pi i/3+i0^+}}^{e^{\pi i/3+i0^+}} \right) \left[\text{Li}_r \left(\frac{2z^3}{(1+z^3)^2} \right) \log \frac{2z^3}{(1+z^3)^2} \right] R_{12}(z) \frac{dz}{2\pi i} \end{aligned}$$

holds for $\delta \in (0, 1)$. Thus, the branch cut of $\log \frac{2z^3}{(1+z^3)^2}$ eventually forms a term in the \mathbb{Q} -vector space $\mathfrak{Z}_{r+1}(12) + \sqrt{3}\mathfrak{Z}_{r+1}(12)$ after contour integration, according to GPL recursion and (1.3''). In all, the difference between the right-hand sides of (1.12) and (1.14) is ascribed to the participation of yet another GPL shuffling (3.4), which increases the weight from r to $r+1$.

The identity (1.15) is a special case of the procedures to be expounded in Section 3.3.

What remains to be checked is (1.13). In place of (1.12*), we now have

$$\begin{aligned} & \sum_{k=0}^{\infty} \frac{2^k \binom{3k}{k}}{3^{3k}} \text{H}_{2k}^{(r)} \\ &= \left(\int_0^{\infty} + \int_{\infty e^{2\pi i/3}}^0 \right) \left[\text{Li}_r \left(\frac{\sqrt{2}z^3}{1+z^6} \right) R_{24}^+(z) + \text{Li}_r \left(-\frac{\sqrt{2}z^3}{1+z^6} \right) R_{24}^-(z) \right] \frac{dz}{2\pi i}, \quad (1.13^*) \end{aligned}$$

where the rational functions

$$R_{24}^{\pm}(z) := \frac{3\sqrt{3}i}{2} \left(\frac{1}{1-e^{4\pi i/3}} + \frac{z^2}{1-e^{2\pi i/3}} \right) \frac{1}{1 \mp \frac{\sqrt{2}z^3}{1+z^6}} \frac{z}{1+z^3}$$

have only simple poles at certain 24th roots of unity. Furthermore, the residues at these poles all belong to $\mathbb{Q} + \mathbb{Q}\sqrt{3}$. Subsequent branch cut analyses and GPL fibrations of (1.13*) then complete the proof of (1.13). \blacksquare

We can now transfer the procedures above to the analysis of Sun's series involving $\binom{4k}{2k}$.

Proof of Theorem 1.3(c) for $\mathfrak{Z}_k(16)$ and $\mathfrak{Z}_k(24)$, where $k \in \mathbb{Z}_{>1}$. For the verification of equation (1.16), consider

$$\sum_{k=0}^{\infty} \frac{\binom{4k}{2k}}{2^{5k}} \text{H}_k^{(r)} = \left(\int_{i\infty}^0 + \int_0^{\infty} \right) \text{Li}_r \left(\frac{2z^4}{(1+z^4)^2} \right) R_{16}(z) \frac{dz}{2\pi i}, \quad (1.16^*)$$

where the rational function

$$R_{16}(z) := 2\sqrt{2}i \left(\frac{1}{1-i} + \frac{z^2}{1+i} \right) \frac{1}{1 - \frac{2z^4}{(1+z^4)^2}} \frac{1}{1+z^4}$$

has only simple poles at certain 16th roots of unity, with residues in the \mathbb{Q} -vector space

$$\mathbb{Q}\sqrt{1 + \frac{1}{\sqrt{2}}} + \mathbb{Q}\sqrt{1 - \frac{1}{\sqrt{2}}}.$$

One can thus deform the contour in (1.16*) to a tight loop $C_\varepsilon^{[\pi/8, 3\pi/8]}$ wrapping around the branch cut of the polylogarithm, as done in the proof of Theorem 1.3 (b).

The rationale behind (1.17) is similar. ■

3.3 Logarithmic forms of Sun's series

In [23, Section 3], not only have we specified critical parameters in infinite series that produce CMZV evaluations, we have also investigated the “inverse binomial sums” and “binomial sums” involving $\binom{2k}{k}$ and generic parameters, such as those on the right-hand sides of (1.18)–(1.19).

In this subsection, we examine some convergent series involving $\binom{3k}{k}$ and $\binom{4k}{2k}$, in the general setting of Theorem 1.7.

Proof of Theorem 1.7 (a). According to our experience in Section 3.2, we have the following companions to (1.20) for $|1 + \Xi^3|^2 < 4|\Xi^3|$:

$$\begin{aligned} & \frac{3\sqrt{3}}{2\pi} \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^\infty \right) \frac{\text{Li}_1 \left(\frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2} \right)}{1 - \frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2}} \frac{dz}{1+z^3} \\ &= (1 - e^{2\pi i/3}) \sum_{k=0}^\infty \frac{\binom{3k}{k}}{3^{3k}} \left[\frac{(1 + \Xi^3)^2}{\Xi^3} \right]^k \mathbf{H}_k, \end{aligned} \quad (1.20^\circ)$$

$$\begin{aligned} & \frac{3\sqrt{3}}{2\pi} \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^\infty \right) \frac{\text{Li}_1 \left(\frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2} \right)}{1 - \frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2}} \frac{z dz}{1+z^3} \\ &= (1 - e^{4\pi i/3}) \sum_{k=0}^\infty \frac{\binom{3k}{k}}{3^{3k}} \left[\frac{(1 + \Xi^3)^2}{\Xi^3} \right]^k \mathbf{H}_k, \end{aligned} \quad (1.20^\dagger)$$

$$\frac{3\sqrt{3}}{2\pi} \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^\infty \right) \frac{\text{Li}_1 \left(\frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2} \right)}{1 - \frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2}} \frac{z^2 dz}{1+z^3} = 0. \quad (1.20^\ddagger)$$

If we also know that $\arg \Xi \in (0, 2\pi/3)$, then each individual integrand here has two simple poles (namely Ξ and $e^{2\pi i/3}/\Xi$) in the sector $\arg z \in (0, 2\pi/3)$. We can take a certain \mathbb{C} -linear combination of the last three displayed equations, so that the resulting integrand is free from simple poles within the same sector:

$$\begin{aligned} & \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^\infty \right) \frac{\text{Li}_1 \left(\frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2} \right)}{1 - \frac{z^3(1+\Xi^3)^2}{\Xi^3(1+z^3)^2}} \frac{3\sqrt{3}i(z - \Xi)(z - e^{2\pi i/3}/\Xi)}{1+z^3} \frac{dz}{2\pi i} \\ &= \left[\frac{3}{2} \left(\frac{1}{\Xi} - \Xi \right) - \frac{i\sqrt{3}}{2} \left(\Xi + \frac{1}{\Xi} \right) + i\sqrt{3} \right] \sum_{k=0}^\infty \frac{\binom{3k}{k}}{3^{3k}} \left[\frac{(1 + \Xi^3)^2}{\Xi^3} \right]^k \mathbf{H}_k. \end{aligned} \quad (1.20^\heartsuit)$$

As we specialize (1.20[♥]) to $\Xi = e^{i\varphi}$ for $\varphi \in (0, \pi/3)$, and deform the contour of integration, we get

$$\sum_{k=0}^\infty \frac{\binom{3k}{k}}{3^{3k}} \left(4 \cos^2 \frac{3\varphi}{2} \right)^k \mathbf{H}_k = \lim_{\varepsilon \rightarrow 0^+} \int_{C_\varepsilon^{[\varphi, 2\pi/3-\varphi]}} \text{Li}_1 \left(\frac{4z^3 \cos^2 \frac{3\varphi}{2}}{(1+z^3)^2} \right) R_\varphi^\Delta(z) \frac{dz}{2\pi i}, \quad (1.20^\Delta)$$

where

$$R_\varphi^\Delta(z) := \frac{\sqrt{3}i \sin \left(\frac{\varphi}{2} - \frac{2\pi}{3} \right)}{\sin^2 \frac{3\varphi}{2}} \left[\frac{e^{\frac{i\varphi}{2} - \frac{\pi i}{3}} \sin \varphi}{z - e^{i\varphi + \frac{2\pi i}{3}}} - \frac{e^{\frac{i\varphi}{2}} \sin \left(\varphi + \frac{\pi}{3} \right)}{z - e^{i\varphi - \frac{2\pi i}{3}}} \right]$$

$$\left. - \frac{e^{-\frac{i\varphi}{2} + \frac{\pi i}{3}} \sin \varphi}{z - e^{-i\varphi}} + \frac{e^{-\frac{i\varphi}{2}} \sin \left(\varphi + \frac{\pi}{3}\right)}{z - e^{-i\varphi - \frac{2\pi i}{3}}} \right].$$

In view of the branch cut behavior,

$$\lim_{\varepsilon \rightarrow 0^+} \left[\operatorname{Li}_1 \left(\frac{4[(1+\varepsilon)e^{i\phi}]^3 \cos^2 \frac{3\varphi}{2}}{\{1 + [(1+\varepsilon)e^{i\phi}]^3\}^2} \right) - \operatorname{Li}_1 \left(\frac{4[(1-\varepsilon)e^{i\phi}]^3 \cos^2 \frac{3\varphi}{2}}{\{1 + [(1-\varepsilon)e^{i\phi}]^3\}^2} \right) \right] = 2\pi i \frac{\phi - \frac{\pi}{3}}{\left| \phi - \frac{\pi}{3} \right|}$$

for $\phi \in [\varphi, \pi/3) \cup (\pi/3, 2\pi/3 - \varphi]$, we can compute the right-hand side of (1.20^Δ) by integrating four rational functions that are non-singular in a neighborhood of the loop $C_\varepsilon^{[\pi, 2\pi/3 - \varphi]}$, so the final form of (1.20) [given in Theorem 1.7 (a)] emerges after a little trigonometry.

To establish (1.21) in full, we examine

$$\frac{3\sqrt{3}}{2\pi} \left(\int_{\infty e^{2\pi i/3}}^0 + \int_0^\infty \right) \frac{-3 \log z - 2 \log \left(1 + \frac{1}{z^3}\right)}{1 - \frac{4z^3 \cos^2 \frac{3\varphi}{2}}{(1+z^3)^2}} \frac{dz}{1+z^3} \quad (1.21^\circ)$$

in two ways. First, by tracking the integrand literally along the contour above, we see that (1.21[◦]) is equal to

$$\begin{aligned} & \frac{3\sqrt{3}}{2\pi} (1 - e^{2\pi i/3}) \int_0^\infty \frac{\log \frac{z^3}{(1+z^3)^2}}{1 - \frac{4z^3 \cos^2 \frac{3\varphi}{2}}{(1+z^3)^2}} \frac{dz}{1+z^3} + 2\pi i e^{2\pi i/3} \int_0^\infty \frac{1}{1 - \frac{4z^3 \cos^2 \frac{3\varphi}{2}}{(1+z^3)^2}} \frac{dz}{1+z^3} \\ &= (1 - e^{2\pi i/3}) \sum_{k=0}^\infty \frac{\binom{3k}{k}}{3^{3k}} \left(4 \cos^2 \frac{3\varphi}{2}\right)^k (3\mathbf{H}_{3k} - 2\mathbf{H}_{2k} - \mathbf{H}_k - 3 \log 3) \\ & \quad + 2\pi i e^{2\pi i/3} \sum_{k=0}^\infty \frac{\binom{3k}{k}}{3^{3k}} \left(4 \cos^2 \frac{3\varphi}{2}\right)^k, \end{aligned}$$

where the last infinite sum evaluates to $\sin\left(\frac{\varphi}{2} + \frac{\pi}{3}\right) \csc \frac{3\varphi}{2}$ [19, Remark 2.7]. Second, we close the contour in the sector $\arg z \in [0, 2\pi/3]$, taking care of the branch cut that is a straight line segment joining 0 to $e^{\pi i/3}$, while picking up residues at $z = e^{i\varphi}$ and $z = e^{2\pi i/3 - i\varphi}$ in the meantime. The net result then translates into (1.21) as stated in Theorem 1.7 (a).

The proof of (1.22) is similar to that of (1.20). ■

Proof of Theorem 1.7 (b). We have

$$\begin{aligned} \sum_{k=0}^\infty \frac{\binom{4k}{2k}}{2^{6k}} (4 \cos^2 2\psi)^k \mathbf{H}_k &= \frac{2\sqrt{2}}{\pi} \frac{1}{1-i} \left(\int_{i\infty}^0 + \int_0^\infty \right) \frac{\operatorname{Li}_1 \left(\frac{4z^4 \cos^2 2\psi}{(1+z^4)^2} \right)}{1 - \frac{4z^4 \cos^2 2\psi}{(1+z^4)^2}} \frac{dz}{1+z^4} \\ &= \frac{2\sqrt{2}}{\pi} \frac{1}{1+i} \left(\int_{i\infty}^0 + \int_0^\infty \right) \frac{\operatorname{Li}_1 \left(\frac{4z^4 \cos^2 2\psi}{(1+z^4)^2} \right)}{1 - \frac{4z^4 \cos^2 2\psi}{(1+z^4)^2}} \frac{z^2 dz}{1+z^4} \end{aligned}$$

by analogy to (1.20[◦]) and (1.20[†]). Instead of the zero-padding identity in (1.20[†]), we now have a trailing term

$$\begin{aligned} & \frac{2\sqrt{2}}{\pi} \left(\int_{i\infty}^0 + \int_0^\infty \right) \frac{\operatorname{Li}_1 \left(\frac{4z^4 \cos^2 2\psi}{(1+z^4)^2} \right)}{1 - \frac{4z^4 \cos^2 2\psi}{(1+z^4)^2}} \frac{z dz}{1+z^4} = \frac{2\sqrt{2}}{\pi} \int_0^\infty \frac{\operatorname{Li}_1 \left(\frac{4x^2 \cos^2 2\psi}{(1+x^2)^2} \right)}{1 - \frac{4x^2 \cos^2 2\psi}{(1+x^2)^2}} \frac{dx}{1+x^2} \\ &= \sqrt{2} \sum_{k=0}^\infty \frac{\binom{2k}{k}}{2^{4k}} (4 \cos^2 2\psi)^k \mathbf{H}_k = \frac{2\sqrt{2}}{\sin 2\psi} \log \frac{1 + \sin 2\psi}{2 \sin 2\psi}. \end{aligned}$$

Here, in the penultimate step, we have produced binomial coefficients from an integral representation of Euler's beta function [14, item 8.380.3]; in the last step, we have quoted Boyadzhiev's formula [19, formula (1.1)].

According to the information in the last passage, we can construct a relevant analog of (1.20 Δ) in the following form:

$$\begin{aligned} & \sum_{k=0}^{\infty} \frac{\binom{4k}{2k}}{2^{6k}} (4 \cos^2 2\psi)^k \mathbf{H}_k - \frac{2 \sin(\psi + \frac{\pi}{4})}{\sin 2\psi} \log \frac{1 + \sin 2\psi}{2 \sin 2\psi} \\ &= \lim_{\varepsilon \rightarrow 0^+} \int_{C_\varepsilon^{[\psi, \pi/2 - \psi]}} \text{Li}_1 \left(\frac{4z^4 \cos^2 2\psi}{(1+z^4)^2} \right) R_\psi^\square(z) \frac{dz}{2\pi i}, \end{aligned} \quad (1.23^\square)$$

where

$$R_\psi^\square(z) := \frac{\sqrt{2}(1+i)(z - e^{i\psi})(z - ie^{-i\psi})}{1 - \frac{4z^4 \cos^2 2\psi}{(1+z^4)^2}} \frac{1}{1+z^4}.$$

We leave detailed calculations and subsequent arguments behind (1.23 \square) to diligent readers. \blacksquare

Until now, our working examples for CMZVs of levels $N \in \{4, 8, 12, 16, 24\}$ are restricted to constructible cyclotomy, where all the algebraic numbers of our interest can be represented through (nested) square roots. The proofs in the current subsection are by no means limited to regular polygons constructible through ruler and compass.

To illustrate the generality of our methods, we point out that the proofs of Theorems 1.3 (b) and 1.7 (a) can be readily adapted to the following statements for all $r \in \mathbb{Z}_{>0}$:

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \mathbf{H}_k^{(r)} = \frac{3\sqrt{3}}{2\pi} \int_0^\infty \frac{\text{Li}_r\left(\frac{X^3}{(1+X^3)^2}\right)}{1 - \frac{X^3}{(1+X^3)^2}} \frac{dX}{1+X^3} \in c_{2/9}\mathfrak{Z}_r(18) + c_{4/9}\mathfrak{Z}_r(18), \quad (3.5)$$

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{2k}} \mathbf{H}_k^{(r)} = \frac{3\sqrt{3}}{2\pi} \int_0^\infty \frac{\text{Li}_r\left(\frac{3X^3}{(1+X^3)^2}\right)}{1 - \frac{3X^3}{(1+X^3)^2}} \frac{dX}{1+X^3} \in c_{2/9}\mathfrak{Z}_r(9) + c_{4/9}\mathfrak{Z}_r(9), \quad (3.6)$$

where $c_\nu := \cos(\nu\pi)$. Here, if $r \in \{1, 2\}$, then we can sharpen the right-hand side of (3.5) into $c_{2/9}\mathfrak{Z}_r(9) + c_{4/9}\mathfrak{Z}_r(9)$ by Au's automated reduction [7] of the corresponding GPL output.

Defining further $s_\nu := \sin(\nu\pi)$ and $\lambda_\nu := \log(2s_\nu)$, we have the following instances of (3.5) and (3.6):

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \mathbf{H}_k = -2(3c_{2/9} + 2c_{4/9})\lambda_{1/9} - 2(2c_{2/9} + 5c_{4/9})\lambda_{2/9} + 2(c_{4/9} - c_{2/9})\lambda_{1/3},$$

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{2k}} \mathbf{H}_k = -6(c_{2/9} + c_{4/9})\lambda_{1/9} + 6c_{2/9}\lambda_{2/9} - 2(2c_{2/9} + c_{4/9})\lambda_{1/3},$$

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{3k}} \mathbf{H}_k^{(2)} &= 12(c_{2/9} + 3c_{4/9}) \text{Li}_2(2c_{4/9}) - 18(c_{2/9} + 2c_{4/9}) \text{Li}_2(4c_{4/9}^2) \\ &\quad - 18c_{4/9} \text{Li}_2\left(\frac{4}{3}s_{1/9}^2\right) - 6c_{4/9}(\lambda_{1/9}^2 - 2\lambda_{1/9}\lambda_{2/9} - 2\lambda_{2/9}^2 + \lambda_{1/3}^2) \\ &\quad - 12c_{4/9}(2\lambda_{1/9} + \lambda_{2/9})\lambda_{1/3} - \frac{2(c_{2/9} + 3c_{4/9})\pi^2}{9}, \end{aligned}$$

$$\sum_{k=0}^{\infty} \frac{\binom{3k}{k}}{3^{2k}} \mathbf{H}_k^{(2)} = -12(c_{2/9} - c_{4/9}) \text{Li}_2(2c_{4/9}) + 12(c_{2/9} - c_{4/9}) \text{Li}_2(4c_{4/9}^2)$$

$$+ 12c_{2/9} \operatorname{Li}_2 \left(\frac{4}{3} s_{1/9}^2 \right) + 6c_{2/9} (\lambda_{1/9} + \lambda_{1/3})^2 + \frac{2(c_{2/9} - c_{4/9})\pi^2}{9},$$

and the list goes on.

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References

- [1] Ablinger J., Discovering and proving infinite binomial sums identities, *Exp. Math.* **26** (2017), 62–71, [arXiv:1507.01703](#).
- [2] Ablinger J., Discovering and proving infinite Pochhammer sum identities, *Exp. Math.* **31** (2022), 309–323, [arXiv:1902.11001](#).
- [3] Ablinger J., Blümlein J., Raab C.G., Schneider C., Iterated binomial sums and their associated iterated integrals, *J. Math. Phys.* **55** (2014), 112301, 57 pages, [arXiv:1407.1822](#).
- [4] Ablinger J., Blümlein J., Schneider C., Harmonic sums and polylogarithms generated by cyclotomic polynomials, *J. Math. Phys.* **52** (2011), 102301, 52 pages, [arXiv:1105.6063](#).
- [5] Ablinger J., Blümlein J., Schneider C., Analytic and algorithmic aspects of generalized harmonic sums and polylogarithms, *J. Math. Phys.* **54** (2013), 082301, 74 pages, [arXiv:1302.0378](#).
- [6] Au K.C., Evaluation of one-dimensional polylogarithmic integral, with applications to infinite series, [arXiv:2007.03957](#).
- [7] Au K.C., Iterated integrals and multiple polylogarithm at algebraic arguments, [arXiv:2201.01676](#), Software available at https://www.researchgate.net/publication/357601353_Mathematica_package_MultipleZetaValues and <https://www.wolframcloud.com/obj/pisco125/MultipleZetaValues-1.2.0.paclet>.
- [8] Charlton S., Gangl H., Lai L., Xu C., Zhao J., On two conjectures of Sun concerning Apéry-like series, *Forum Math.*, to appear, [arXiv:2210.14704](#).
- [9] Davydychev A.I., Kalmykov M.Yu., New results for the ε -expansion of certain one-, two- and three-loop Feynman diagrams, *Nuclear Phys. B* **605** (2001), 266–318, [arXiv:hep-th/0012189](#).
- [10] Davydychev A.I., Kalmykov M.Yu., Massive Feynman diagrams and inverse binomial sums, *Nuclear Phys. B* **699** (2004), 3–64, [arXiv:hep-th/0303162](#).
- [11] Frellesvig H., Tommasini D., Wever C., On the reduction of generalized polylogarithms to Li_n and $\operatorname{Li}_{2,2}$ and on the evaluation thereof, *J. High Energy Phys.* **2016** (2016), no. 3, 189, 35 pages, [arXiv:1601.02649v3](#).
- [12] Goncharov A.B., The double logarithm and Manin's complex for modular curves, *Math. Res. Lett.* **4** (1997), 617–636.
- [13] Goncharov A.B., Multiple polylogarithms, cyclotomy and modular complexes, *Math. Res. Lett.* **5** (1998), 497–516, [arXiv:1105.2076](#).
- [14] Gradshteyn I.S., Ryzhik I.M., Table of integrals, series, and products, Elsevier, Amsterdam, 2007.
- [15] Kalmykov M.Yu., Veretin O., Single-scale diagrams and multiple binomial sums, *Phys. Lett. B* **483** (2000), 315–323, [arXiv:hep-th/0004010](#).
- [16] Kalmykov M.Yu., Ward B.F.L., Yost S.A., Multiple (inverse) binomial sums of arbitrary weight and depth and the all-order ε -expansion of generalized hypergeometric functions, *J. High Energy Phys.* **2007** (2007), no. 10, 048, 26 pages, [arXiv:0707.3654](#).

-
- [17] Mező I., Nonlinear Euler sums, *Pacific J. Math.* **272** (2014), 201–226.
 - [18] Panzer E., Algorithms for the symbolic integration of hyperlogarithms with applications to Feynman integrals, *Comput. Phys. Commun.* **188** (2015), 148–166, [arXiv:1403.3385](#).
 - [19] Sun Z.-W., Series with summands involving harmonic numbers, in Combinatorial and Additive Number Theory, to appear, [arXiv:2210.07238v8](#).
 - [20] Weinzierl S., Expansion around half-integer values, binomial sums, and inverse binomial sums, *J. Math. Phys.* **45** (2004), 2656–2673, [arXiv:hep-ph/0402131](#).
 - [21] Xu C., Zhao J., Sun’s three conjectures on Apéry-like sums involving harmonic numbers, 2022, [arXiv:2203.04184](#).
 - [22] Xu C., Zhao J., A note on Sun’s conjectures on Apéry-like sums involving Lucas sequences and harmonic numbers, [arXiv:2204.08277](#).
 - [23] Zhou Y., Hyper-Mahler measures via Goncharov–Deligne cyclotomy, [arXiv:2210.17243v3](#).