Research Article

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On two conjectures of Sun concerning Apéry-like series

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Abstract: We prove two conjectural identities of Z.-W. Sun concerning Apéry-like series. One of the series is alternating, whereas the other one is not. Our main strategy is to convert the series and the alternating series to log-sine-cosine and log-sinh-cosh integrals, respectively. Then we express all these integrals using single-valued Bloch–Wigner–Ramakrishnan–Wojtkowiak–Zagier polylogarithms. The conjectures then follow from a few rather non-trivial functional equations of those polylogarithms in weights 3 and 4.

Keywords: Apéry-like series, log-sine-cosine integrals, colored multiple zeta values, Sun's conjectures

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1 Introduction

Let $\zeta(s) := \sum_{n=1}^{\infty} n^{-s}$ be the Riemann zeta function for Re $s > 1$. In the 1979's proof [1] of the irrationality of $\zeta(3)$, R. Apéry made use of the following infinite series involving central binomial coefficients:

$$\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^3\binom{2n}{n}} = \frac{2}{5}\zeta(3).$$

Since then, the *Apéry-like* series have attracted much attention, and many tools and theories have been developed to evaluate these series in closed forms. For example, Cantarini and D'Aurizio [6] studied a few families of Apéry-like series involving central binomial coefficients and their higher powers by computing the Fourier–Legendre expansions of $\log(x)/\sqrt{x}$ and related functions, and by applying suitable transformation formulas to certain (twisted) hypergeometric series. We refer the reader to [14] for a more comprehensive and detailed survey on recent progress.

The aim of this paper is to prove two conjectures of Z.-W. Sun concerning Apéry-like series. These conjectures were published first in [11] and included in Sun's book [12]. Define the classical harmonic numbers

$$H_n := \sum_{k=1}^{n} \frac{1}{k} \quad \text{for } n = 1, 2, 3, \ldots.$$

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Let

$$\beta(s) := \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^s} \quad \text{for } \operatorname{Re} s > 0$$

be the Dirichlet beta function.

Conjecture 1.1 ([12, Conjectures 10.59 (i) and 10.60]). *We have*

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{(2n+1)^3 16^n}\left(9H_{2n+1} + \frac{32}{2n+1}\right) = 40\beta(4) + \frac{5}{12}\pi\zeta(3), \tag{1.1}$$

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{(2n+1)^2(-16)^n}\left(5H_{2n+1} + \frac{12}{2n+1}\right) = 14\zeta(3). \tag{1.2}$$

There are two major steps in our proof of these conjectured identities. First we will express the Apéry-type series on the left-hand side of (1.1) and (1.2) by some log-sine-cosine and log-sinh-cosh integrals respectively. Then we will evaluate these integrals using a single-valued version of the polylogarithms, denoted by $\widetilde{D}_m(x)$ in Zagier's seminal paper [16].

2 Log-sine-cosine integrals

Definition 2.1. Let j and k be two positive integers. For any real number θ, we define the *log-sine integrals* by

$$\mathrm{Ls}_j(\theta) := -\int_0^{\theta} \log^{j-1}\left|2\sin\frac{t}{2}\right| \mathrm{d}t,$$

and more generally, the *log-sine-cosine integrals* by

$$\mathrm{Lsc}_{j,k}(\theta) := -\int_0^{\theta} \log^{j-1}\left|2\sin\frac{t}{2}\right| \log^{k-1}\left|2\cos\frac{t}{2}\right| \mathrm{d}t.$$

Similarly, for any real number θ, we define the *log-sinh integrals* by

$$\mathrm{Lsh}_j(\theta) := -\int_0^{\theta} \log^{j-1}\left|2\sinh\frac{t}{2}\right| \mathrm{d}t,$$

and more generally, the *log-sinh-cosh integrals* by

$$\mathrm{Lshch}_{j,k}(\theta) := -\int_0^{\theta} \log^{j-1}\left|2\sinh\frac{t}{2}\right| \log^{k-1}\left|2\cosh\frac{t}{2}\right| \mathrm{d}t.$$

The log-sine-cosine integrals have been considered by L. Lewin [9, 10]. They appear in physical applications as well; see for instance [7].

The following simple fact is useful. For any positive integers p and n, and for any nonnegative real number z, we have

$$\frac{1}{(p-1)!}\int_0^{z} \frac{\log^{p-1}(\frac{z}{w})}{w} \cdot w^n \,\mathrm{d}w = \frac{z^n}{n^p}. \tag{2.1}$$

Lemma 2.1. *For any nonnegative integer p and real number $z \in [0, \frac{1}{2}]$, we have*

$$\sum_{n=0}^{\infty} \binom{2n}{n} \frac{z^{2n+1}}{(2n+1)^{p+1}} = \frac{\theta}{2}\frac{\log^p(2\sin\theta)}{p!} + \frac{1}{4p!}\sum_{j=1}^{p}(-1)^{j-1}\binom{p}{j}\log^{p-j}(2\sin\theta)\,\mathrm{Ls}_{j+1}(2\theta), \tag{2.2}$$

where $\theta := \arcsin(2z) \in [0, \frac{\pi}{2}]$.

Similarly, for any nonnegative integer p and real number $z \in [0, \frac{1}{2}]$, *we have*

$$\sum_{n=0}^{\infty} \binom{2n}{n} \frac{(-1)^n z^{2n+1}}{(2n+1)^{p+1}} = \frac{\theta}{2} \frac{\log^p(2\sinh\theta)}{p!} + \frac{1}{4p!} \sum_{j=1}^{p} (-1)^{j-1} \binom{p}{j} \log^{p-j}(2\sinh\theta) \operatorname{Lsh}_{j+1}(2\theta), \tag{2.3}$$

where $\theta := \operatorname{arcsinh}(2z) \in [0, \log(\sqrt{2}+1)]$.

Proof. The first identity (2.2) is proved in [5, Theorem 4]. For (2.3), we start with the simple identity

$$\sum_{n=0}^{\infty} \binom{2n}{n} (-1)^n z^{2n+1} = \frac{z}{\sqrt{1+4z^2}} = \frac{\tanh\theta}{2} \quad \left(\text{recall } z = \frac{1}{2}\sinh\theta\right).$$

By (2.1), we have

$$\begin{aligned}
\sum_{n=0}^{\infty} \binom{2n}{n} \frac{(-1)^n z^{2n+1}}{(2n+1)^{p+1}} &= \frac{1}{p!} \int_0^z \frac{\log^p(\frac{z}{w})}{w} \cdot \sum_{n=0}^{\infty} \binom{2n}{n} (-1)^n w^{2n+1}\, dw \\
&= \frac{1}{p!} \int_0^\theta \frac{\log^p(\frac{1}{2}\sinh\theta / \frac{1}{2}\sinh t)}{\frac{1}{2}\sinh t} \cdot \frac{\tanh t}{2}\, d\left(\frac{1}{2}\sinh t\right) \quad \left(w = \frac{1}{2}\sinh t\right) \\
&= \frac{1}{2p!} \int_0^\theta (\log(2\sinh\theta) - \log(2\sinh t))^p\, dt \\
&= \frac{\theta}{2} \frac{\log^p(2\sinh\theta)}{p!} + \frac{1}{2p!} \sum_{j=1}^{p} (-1)^j \binom{p}{j} \log^{p-j}(2\sinh\theta) \int_0^\theta \log^j(2\sinh t)\, dt \\
&= \frac{\theta}{2} \frac{\log^p(2\sinh\theta)}{p!} + \frac{1}{4p!} \sum_{j=1}^{p} (-1)^{j-1} \binom{p}{j} \log^{p-j}(2\sinh\theta) \operatorname{Lsh}_{j+1}(2\theta).
\end{aligned}$$

The proof is now complete. □

Lemma 2.2. *For any positive integer p and real number* $z \in [0, \frac{1}{2}]$, *we have*

$$\begin{aligned}
\sum_{n=1}^{\infty} \binom{2n}{n} \frac{H_{2n}}{(2n+1)^p} z^{2n+1} &= \frac{1}{(p-1)!} \sum_{j=1}^{p} (-1)^{j-1} \binom{p-1}{j-1} \log^{p-j}(2\sin\theta) \\
&\quad \times \left\{ \frac{1}{2} \operatorname{Lsc}_{j,2}(2\theta) - \sum_{l=1}^{j} \binom{j-1}{l-1} \operatorname{Lsc}_{l,j-l+2}(\theta) \right\},
\end{aligned} \tag{2.4}$$

where $\theta = \arcsin(2z) \in [0, \frac{\pi}{2}]$.

Similarly, for any positive integer p and real number $z \in [0, \frac{1}{2}]$, *we have*

$$\begin{aligned}
\sum_{n=1}^{\infty} \binom{2n}{n} \frac{H_{2n}}{(2n+1)^p} (-1)^n z^{2n+1} &= \frac{1}{(p-1)!} \sum_{j=1}^{p} (-1)^{j-1} \binom{p-1}{j-1} \log^{p-j}(2\sinh\theta) \\
&\quad \times \left\{ \frac{1}{2} \operatorname{Lshch}_{j,2}(2\theta) - \sum_{l=1}^{j} \binom{j-1}{l-1} \operatorname{Lshch}_{l,j-l+2}(\theta) \right\},
\end{aligned} \tag{2.5}$$

where $\theta = \operatorname{arcsinh}(2z) \in [0, \log(\sqrt{2}+1)]$.

Proof. We first prove (2.4). By [7, equation (D.8), pp. 52–53], we have

$$\sum_{n=1}^{\infty} \binom{2n}{n} \frac{z^n}{2n} = \log(1+\chi), \qquad \sum_{n=1}^{\infty} \binom{2n}{n} H_{2n-1} z^n = \frac{2}{1-\chi} [\chi \log(1+\chi) - (1+\chi)\log(1-\chi)],$$

where $\chi := \frac{1-\sqrt{1-4z}}{1+\sqrt{1-4z}}$. Summing up the two equations, substituting z^2 for z and then multiplying by z, we obtain

$$\sum_{n=1}^{\infty} \binom{2n}{n} H_{2n} z^{2n+1} = \frac{z}{\sqrt{1-4z^2}} \left(\log\left(\frac{2}{1+\sqrt{1-4z^2}}\right) - 2\log\left(\frac{2\sqrt{1-4z^2}}{1+\sqrt{1-4z^2}}\right) \right). \tag{2.6}$$

By the change of variables $z = \frac{1}{2}\sin\theta$ for $z \in [0, \frac{1}{2})$ and $\theta \in [0, \frac{\pi}{2})$, we arrive at

$$\sum_{n=1}^{\infty}\binom{2n}{n}H_{2n}z^{2n+1} = \tan\theta \cdot \Big(\log\Big(2\cos\frac{\theta}{2}\Big) - \log(2\cos\theta)\Big).$$

Using (2.1), we obtain

$$\begin{aligned}\sum_{n=1}^{\infty}\binom{2n}{n}\frac{H_{2n}}{(2n+1)^p}z^{2n+1} &= \frac{1}{(p-1)!}\int_0^z \frac{\log^{p-1}(\frac{z}{w})}{w}\cdot\sum_{n=1}^{\infty}\binom{2n}{n}H_{2n}w^{2n+1}\,\mathrm{d}w \\ &= \frac{1}{(p-1)!}\int_0^\theta (\log(2\sin\theta) - \log(2\sin t))^{p-1} \\ &\qquad \cdot\Big(\log\Big(2\cos\frac{t}{2}\Big) - \log(2\cos t)\Big)\,\mathrm{d}t \quad \Big(w = \frac{1}{2}\sin t\Big) \\ &= \frac{1}{(p-1)!}\sum_{j=1}^{p}(-1)^{j-1}\binom{p-1}{j-1}\log^{p-j}(2\sin\theta) \\ &\qquad \times\int_0^\theta \log^{j-1}(2\sin t)\cdot\Big(\log\Big(2\cos\frac{t}{2}\Big) - \log(2\cos t)\Big)\,\mathrm{d}t. \end{aligned} \tag{2.7}$$

We observe that

$$\int_0^\theta \log^{j-1}(2\sin t)\cdot(-\log(2\cos t))\,\mathrm{d}t = \frac{1}{2}\,\mathrm{Lsc}_{j,2}(2\theta), \tag{2.8}$$

$$\begin{aligned}\int_0^\theta \log^{j-1}(2\sin t)\cdot\log\Big(2\cos\frac{t}{2}\Big)\,\mathrm{d}t &= \int_0^\theta\Big(\log\Big(2\sin\frac{t}{2}\Big) + \log\Big(2\cos\frac{t}{2}\Big)\Big)^{j-1}\cdot\log\Big(2\cos\frac{t}{2}\Big)\,\mathrm{d}t \\ &= \int_0^\theta\sum_{l=1}^{j}\binom{j-1}{l-1}\log^{l-1}\Big(2\sin\frac{t}{2}\Big)\log^{j-l+1}\Big(2\cos\frac{t}{2}\Big)\,\mathrm{d}t \\ &= -\sum_{l=1}^{j}\binom{j-1}{l-1}\mathrm{Lsc}_{l,j-l+2}(\theta). \end{aligned} \tag{2.9}$$

Inserting (2.8) and (2.9) in (2.7), we complete the proof of (2.4) for $z \in [0, \frac{1}{2})$. The case $z = \frac{1}{2}$ follows from continuity.

The proof of (2.5) is similar. In fact, note that (2.6) is valid for all complex numbers z with $|z| < \frac{1}{2}$. If we substitute $\mathrm{i}z$ for z in (2.6), we have

$$\sum_{n=1}^{\infty}\binom{2n}{n}H_{2n}(-1)^n z^{2n+1} = \frac{z}{\sqrt{1+4z^2}}\Big(\log\Big(\frac{2}{1+\sqrt{1+4z^2}}\Big) - 2\log\Big(\frac{2\sqrt{1+4z^2}}{1+\sqrt{1+4z^2}}\Big)\Big).$$

Letting $z = \frac{1}{2}\sinh\theta$ for $z \in [0, \frac{1}{2})$ and $\theta \in [0, \log(\sqrt{2}+1))$, the above equation can be written as

$$\sum_{n=1}^{\infty}\binom{2n}{n}H_{2n}(-1)^n z^{2n+1} = \tanh\theta\cdot\Big(\log\Big(2\cosh\frac{\theta}{2}\Big) - \log(2\cosh\theta)\Big).$$

Therefore,

$$\begin{aligned}\sum_{n=1}^{\infty}\binom{2n}{n}\frac{H_{2n}}{(2n+1)^p}(-1)^n z^{2n+1} &= \frac{1}{(p-1)!}\int_0^z\frac{\log^{p-1}(\frac{z}{w})}{w}\cdot\sum_{n=1}^{\infty}\binom{2n}{n}H_{2n}(-1)^n w^{2n+1}\,\mathrm{d}w \\ &= \frac{1}{(p-1)!}\int_0^\theta(\log(2\sinh\theta) - \log(2\sinh t))^{p-1} \\ &\qquad \cdot\Big(\log\Big(2\cosh\frac{t}{2}\Big) - \log(2\cosh t)\Big)\,\mathrm{d}t \end{aligned}$$

by the substitution $w = \frac{1}{2}\sinh t$. Identity (2.5) follows from expanding $(\log(2\sinh\theta) - \log(2\sinh t))^{p-1}$ by the binomial theorem. □

3 Proof of (1.1)

Setting $p = 3$ and $z = \frac{1}{4}$ in (2.2) and (2.4), we have $\theta = \frac{\pi}{6}$ and

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{(2n+1)^4 16^n} = \frac{1}{6} \operatorname{Ls}_4\left(\frac{\pi}{3}\right), \tag{3.1}$$

$$\sum_{n=1}^{\infty} \frac{\binom{2n}{n} H_{2n}}{(2n+1)^3 16^n} = \operatorname{Lsc}_{3,2}\left(\frac{\pi}{3}\right) - 2\operatorname{Lsc}_{3,2}\left(\frac{\pi}{6}\right) - 4\operatorname{Lsc}_{2,3}\left(\frac{\pi}{6}\right) - 2\operatorname{Lsc}_{1,4}\left(\frac{\pi}{6}\right). \tag{3.2}$$

For ease of reading, we now outline our proof as the calculations are somewhat involved. We first express the functions $\operatorname{Lsc}_{j,k}(\theta)$ ($j + k = 5$) for $j < k$ in terms of the ones with $j > k$ and then show that we can rewrite each of the latter, after subtracting a suitable linear term in θ, in terms of the single-valued function $\widetilde{D}_4$ (Lemmas 3.3 and 3.4). Substituting $\theta = \frac{\pi}{6}$ and $= \frac{5\pi}{6}$ as in (3.23)–(3.25) then reveals that the ensuing rational multiples of $\pi\zeta(3)$ indeed conspire to match the one on the RHS of (1.1). Moreover, upon realizing that $\beta(4)$ can be written as $\widetilde{D}_4(\mathrm{i})$, the conjectured formula in (1.1) is reduced to showing the vanishing of a rational linear combination of only $\widetilde{D}_4$-terms as in (3.26). It then remains to find – and in fact to concoct – suitable functional equations for $\widetilde{D}_4$ which, after an appropriate specialization, match precisely this combination.

Step 1. It is clear from the definition that

$$\operatorname{Lsc}_{j,k}(\theta) = \operatorname{Lsc}_{j,k}(\pi) - \operatorname{Lsc}_{k,j}(\pi - \theta), \quad \theta \in [0, \pi].$$

The special values of $\operatorname{Lsc}_{j,k}$ at π have been determined by L. Lewin in [9] and [10, Section 7.9]. As observed in [3], Lewin's result can be stated in the form

$$-\frac{1}{\pi} \sum_{m,n=0}^{\infty} \operatorname{Lsc}_{m+1,n+1}(\pi) \frac{x^m}{m!} \frac{y^n}{n!} = \frac{2^{x+y}}{\pi} \frac{\Gamma(\frac{1+x}{2})\Gamma(\frac{1+y}{2})}{\Gamma(1 + \frac{x+y}{2})}.$$

In particular, it is known that

$$\operatorname{Lsc}_{1,4}(\theta) = -\operatorname{Ls}_4(\pi - \theta) + \operatorname{Ls}_4(\pi), \qquad \operatorname{Ls}_4(\pi) = \frac{3}{2}\pi\zeta(3), \tag{3.3}$$

$$\operatorname{Lsc}_{2,3}(\theta) = -\operatorname{Lsc}_{3,2}(\pi - \theta) + \operatorname{Lsc}_{3,2}(\pi), \quad \operatorname{Lsc}_{3,2}(\pi) = -\frac{1}{4}\pi\zeta(3). \tag{3.4}$$

Inserting (3.3) and (3.4) in (3.2), we have

$$\sum_{n=1}^{\infty} \frac{\binom{2n}{n} H_{2n}}{(2n+1)^3 16^n} = 2\operatorname{Ls}_4\left(\frac{5\pi}{6}\right) + \operatorname{Lsc}_{3,2}\left(\frac{\pi}{3}\right) - 2\operatorname{Lsc}_{3,2}\left(\frac{\pi}{6}\right) + 4\operatorname{Lsc}_{3,2}\left(\frac{5\pi}{6}\right) - 2\pi\zeta(3). \tag{3.5}$$

Step 2. We introduce two different versions of the Bloch–Wigner–Ramakrishnan–Wojtkowiak–Zagier polylogarithm [13, 15, 16]: for $|x| \le 1$, $x \ne 0, 1$,

$$D_m(x) = \Re_m\left(\sum_{j=0}^{m} \frac{(-\log|x|)^{m-j}}{(m-j)!} \operatorname{Li}_j(x)\right), \tag{3.6}$$

$$\begin{aligned}\widetilde{D}_m(x) &= D_m(x) + (1 - (-1)^m)\frac{\log^{m-1}|x|}{4 \cdot m!}(2\log|1-x| - \log|x|) \\ &= \Re_m\left(\sum_{j=1}^{m} \frac{(-\log|x|)^{m-j}}{(m-j)!} \operatorname{Li}_j(x) + \frac{\log^{m-1}|x|}{m!} \log|1-x|\right),\end{aligned} \tag{3.7}$$

where $\Re_m = \operatorname{Im}$ for m even and $\Re_m = \operatorname{Re}$ for m odd, and where we adopt Zagier's ad hoc convention $\operatorname{Li}_0(x) \equiv -\frac{1}{2}$ (see [16, p. 413]). It is easy to see that

$$\lim_{x \to 0} \widetilde{D}_m(x) = 0. \tag{3.8}$$

We extend $\widetilde{D}_m(x)$ to $\mathbb{C}\setminus\{0,1\}$ as a single-valued and real analytic function by the *inversion relation* (3.9), and we can check that $\widetilde{D}_m(x)$ satisfies the *complex conjugate relation* (3.10) below:

$$\widetilde{D}_m(x) = (-1)^{m-1}\widetilde{D}_m(x^{-1}), \tag{3.9}$$

$$\widetilde{D}_m(x) = (-1)^{m-1}\widetilde{D}_m(\bar{x}). \tag{3.10}$$

In particular, the complex conjugate relation implies that

$$\widetilde{D}_{2m}(x) = 0 \quad \text{for all } x \in \mathbb{R}. \tag{3.11}$$

It also satisfies *distribution relations* as follows: for any positive integer N, we have

$$\widetilde{D}_m(x^N) = N^{m-1}\sum_{j=0}^{N-1}\widetilde{D}_m(xe^{2j\pi\mathrm{i}/N}).$$

Indeed, this follows easily from the fact that, for all $|x| \le 1$ and $1 \le j \le m$, we have

$$\log^{m-j}|x^N|\,\mathrm{Li}_j(x^N) = N^{m-1}\log^{m-j}|x|\sum_{j=0}^{N-1}\mathrm{Li}_j(xe^{2j\pi\mathrm{i}/N}), \quad 1-x^N = \prod_{j=0}^{N-1}(1-xe^{2j\pi\mathrm{i}/N}).$$

The following computational lemma will be used repeatedly below.

Lemma 3.1. *Let $0<\theta<\pi$. Let $f(x)$ be a rational function of x with real coefficients. Set*

$$g_f(\theta) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\theta}\log f(e^{\mathrm{i}\theta}) = \frac{\mathrm{i}e^{\mathrm{i}\theta}f'(e^{\mathrm{i}\theta})}{2f(e^{\mathrm{i}\theta})}, \quad h_f(\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta}\mathrm{Li}_1(f(e^{\mathrm{i}\theta})) = \frac{\mathrm{i}e^{\mathrm{i}\theta}f'(e^{\mathrm{i}\theta})}{1-f(e^{\mathrm{i}\theta})}.$$

For any positive integer m, let $\sigma_m = 2\mathrm{i}$, $\delta_m = 0$ if m is even and $\sigma_m = 2$, $\delta_m = 1$ if m is odd. Then

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\theta}D_m(f(e^{\mathrm{i}\theta})) &= (-1)^m\Big(D_{m-1}(f(e^{\mathrm{i}\theta})) - \mathfrak{R}_{m-1}\frac{\log^{m-1}|f(e^{\mathrm{i}\theta})|}{2(m-1)!}\Big)\frac{g_f(\theta)+g_f(-\theta)}{\mathrm{i}}\\
&\quad + \frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1}}{\sigma_m\cdot(m-1)!}\big(\delta_m(g_f(\theta)-g_f(-\theta)) + h_f(\theta) + (-1)^m h_f(-\theta)\big),\\
\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_m(f(e^{\mathrm{i}\theta})) &= (-1)^m\Big(\widetilde{D}_{m-1}(f(e^{\mathrm{i}\theta})) - \mathfrak{R}_{m-1}\frac{\log^{m-2}|f(e^{\mathrm{i}\theta})|\log|1-f(e^{\mathrm{i}\theta})|}{(m-1)!}\Big)\frac{g_f(\theta)+g_f(-\theta)}{\mathrm{i}}\\
&\quad + \frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1}}{\sigma_m\cdot(m-1)!}(h_f(\theta)+(-1)^m h_f(-\theta)) + \delta_m\frac{\log^{m-1}|f(e^{\mathrm{i}\theta})|}{2\cdot m!}(h_f(-\theta)-h_f(\theta))\\
&\quad + \delta_m\frac{(m-1)\log^{m-2}|f(e^{\mathrm{i}\theta})|\log|1-f(e^{\mathrm{i}\theta})|}{m!}(g_f(\theta)-g_f(-\theta)).
\end{aligned}$$

Proof. By definition, we may rewrite $D_m(f(e^{\mathrm{i}\theta}))$ as

$$D_m(f(e^{\mathrm{i}\theta})) = \sum_{j=0}^{m}\frac{(\frac{1}{2}(-\log f(e^{\mathrm{i}\theta}) - \log f(e^{-\mathrm{i}\theta})))^{m-j}}{(m-j)!}\cdot\frac{\mathrm{Li}_j(f(e^{\mathrm{i}\theta})) - (-1)^m\mathrm{Li}_j(f(e^{-\mathrm{i}\theta}))}{\sigma_m}.$$

Thus we have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\theta}D_m(f(e^{\mathrm{i}\theta})) &= \frac{1}{\sigma_m}\sum_{j=0}^{m-1}\frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1-j}}{(m-1-j)!}(-g_f(\theta)+g_f(-\theta))(\mathrm{Li}_j(f(e^{\mathrm{i}\theta})) - (-1)^m\mathrm{Li}_j(f(e^{-\mathrm{i}\theta})))\\
&\quad + \frac{1}{\sigma_m}\sum_{j=2}^{m}\frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-j}}{(m-j)!}(2g_f(\theta)\mathrm{Li}_{j-1}(f(e^{\mathrm{i}\theta})) + (-1)^m 2g_f(-\theta)\mathrm{Li}_{j-1}(f(e^{-\mathrm{i}\theta})))\\
&\quad + \frac{1}{\sigma_m}\frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1}}{(m-1)!}(h_f(\theta)+(-1)^m h_f(-\theta)).
\end{aligned}$$

Moving the $j = 0$ term in the first sum to the end, setting $j \to j + 1$ in the second sum, and combining like terms, we then arrive at

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\theta} D_m(f(e^{\mathrm{i}\theta})) &= \frac{1}{\sigma_m} \sum_{j=1}^{m-1} \frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1-j}}{(m-1-j)!} (g_f(\theta) + g_f(-\theta))(\mathrm{Li}_j(f(e^{\mathrm{i}\theta})) + (-1)^m \mathrm{Li}_j(f(e^{-\mathrm{i}\theta}))) \\ &\quad + \frac{1}{\sigma_m} \frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1}}{(m-1)!} (\delta_m(g_f(\theta) - g_f(-\theta)) + h_f(\theta) + (-1)^m h_f(-\theta)) \\ &= (-1)^m \sum_{j=1}^{m-1} \frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1-j}}{(m-1-j)!} \mathfrak{R}_{m-1}(\mathrm{Li}_j(f(e^{\mathrm{i}\theta}))) \frac{g_f(\theta) + g_f(-\theta)}{\mathrm{i}} \\ &\quad + \frac{1}{\sigma_m} \frac{(-\log|f(e^{\mathrm{i}\theta})|)^{m-1}}{(m-1)!} (\delta_m(g_f(\theta) - g_f(-\theta)) + h_f(\theta) + (-1)^m h_f(-\theta)).\end{aligned}$$

The expression for D_m in the lemma now follows easily from the defining formula (3.6).

Turning to $\widetilde{D}_m$, we only need to handle the extra term at the end of (3.7). Noticing that

$$2 \log|1 - x| = -\mathrm{Li}_1(x) - \mathrm{Li}_1(\bar{x}),$$

we have

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\log^{m-1}|f(e^{\mathrm{i}\theta})|}{2 \cdot m!} (2 \log|1 - f(e^{\mathrm{i}\theta})| - \log|f(e^{\mathrm{i}\theta})|) \\ &\quad = \frac{\log^{m-2}|f(e^{\mathrm{i}\theta})|}{2 \cdot m!} (2(m-1) \log|1 - f(e^{\mathrm{i}\theta})| - m \log|f(e^{\mathrm{i}\theta})|)(g_f(\theta) - g_f(-\theta)) \\ &\qquad + \frac{\log^{m-1}|f(e^{\mathrm{i}\theta})|}{2 \cdot m!} (h_f(-\theta) - h_f(\theta)).\end{aligned}$$

Now we can complete the proof of the lemma immediately. □

Corollary 3.2. *Let the notation be as above. Put*

$$A = A(\theta) = \log\left|2 \sin \frac{\theta}{2}\right| = \log|1 - e^{\mathrm{i}\theta}|, \quad B = B(\theta) = \log\left|2 \cos \frac{\theta}{2}\right| = \log|1 + e^{\mathrm{i}\theta}|.$$

For any positive integer m, let $a_m^{\pm} = a_m^{\pm}(\theta) = 1$ if m is even, and $a_m^{\pm} = a_m^{\pm}(\theta) = \mathrm{i}(1 \mp e^{\mathrm{i}\theta})/(1 \pm e^{\mathrm{i}\theta})$ if m is odd. Then, for all $m \geq 3$,

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\theta} A(\theta) = -\frac{a_1^-}{2}, \quad \frac{\mathrm{d}}{\mathrm{d}\theta} B(\theta) = -\frac{a_1^+}{2}, \\ &\frac{\mathrm{d}}{\mathrm{d}\theta} \widetilde{D}_m(\pm e^{\mathrm{i}\theta}) = (-1)^m \widetilde{D}_{m-1}(\pm e^{\mathrm{i}\theta}), \\ &\frac{\mathrm{d}}{\mathrm{d}\theta} \widetilde{D}_m(1 \pm e^{\mathrm{i}\theta}) = \frac{(-1)^m}{2} \widetilde{D}_{m-1}(1 \pm e^{\mathrm{i}\theta}) + (1 + (-1)^m) \frac{A_{\pm}^{m-1}}{2 \cdot (m-1)!} \quad (A_+ = B,\ A_- = A), \\ &\frac{\mathrm{d}}{\mathrm{d}\theta} \widetilde{D}_m\left(\frac{1 - e^{\mathrm{i}\theta}}{1 + e^{\mathrm{i}\theta}}\right) = \frac{\delta_m (A - B)^{m-2}}{2 \cdot m!} ((A - B) a_1^+ + (m-1)(\log 2 - B)(a_1^+ - a_1^-)) + \frac{(B - A)^{m-1}}{2 \cdot (m-1)!} a_m^+.\end{aligned}$$

Proof. By simple calculations,

$$f(x) = 1 \pm x : \begin{cases} g_f(\theta) + g_f(-\theta) = \dfrac{\pm \mathrm{i} e^{\mathrm{i}\theta}}{2(1 \pm e^{\mathrm{i}\theta})} + \dfrac{\pm \mathrm{i} e^{-\mathrm{i}\theta}}{2(1 \pm e^{-\mathrm{i}\theta})} = \dfrac{\mathrm{i}}{2}, \\ g_f(\theta) - g_f(-\theta) = \dfrac{\mathrm{d}}{\mathrm{d}\theta}(A \text{ or } B) = -\dfrac{a_1^{\pm}}{2}, \\ h_f(\theta) + h_f(-\theta) = -2\mathrm{i}, \quad h_f(\theta) - h_f(-\theta) = 0, \end{cases}$$

$$f(x) = \frac{1 - x}{1 + x} : \begin{cases} g_f(\theta) + g_f(-\theta) = \dfrac{-\mathrm{i} e^{\mathrm{i}\theta}}{1 - e^{2\mathrm{i}\theta}} + \dfrac{-\mathrm{i} e^{-\mathrm{i}\theta}}{1 - e^{-2\mathrm{i}\theta}} = 0, \\ g_f(\theta) - g_f(-\theta) = \dfrac{\mathrm{d}}{\mathrm{d}\theta}(A(\theta) - B(\theta)) = \dfrac{a_1^+}{2} - \dfrac{a_1^-}{2}, \\ h_f(\theta) + h_f(-\theta) = \mathrm{i}, \quad h_f(\theta) - h_f(-\theta) = a_1^+. \end{cases}$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_m(1\pm e^{\mathrm{i}\theta}) = \frac{(-1)^m}{2}\widetilde{D}_{m-1}(1\pm e^{\mathrm{i}\theta}) + (1+(-1)^m)\frac{\log^{m-1}|1\pm e^{\mathrm{i}\theta}|}{2\cdot(m-1)!},$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_m\Big(\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big) = \Big(-\log\Big|\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big|\Big)^{m-1}\cdot\frac{h_f(\theta)+(-1)^m h_f(-\theta)}{(m-1)!\cdot\sigma_m} + \frac{\delta_m a_1^+}{2\cdot m!}\log^{m-1}\Big|\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big|$$
$$+\frac{\delta_m}{2m!}(m-1)\log^{m-2}\Big|\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big|\log\Big|\frac{2}{1+e^{\mathrm{i}\theta}}\Big|(a_1^+-a_1^-).$$

These quickly lead to the equalities in the corollary. □

Step 3. Next, we express both Ls_4 and $\mathrm{Lsc}_{3,2}$ in terms of polylogarithms.

Lemma 3.3. *The following expression for* $\mathrm{Ls}_4(\theta)$ *holds for all* $\theta\in(0,\pi)$*:*

$$\mathrm{Ls}_4(\theta) = \frac{3}{2}\zeta(3)\theta + \frac{3}{2}\{-\widetilde{D}_4(e^{\mathrm{i}\theta}) - 4\widetilde{D}_4(1-e^{\mathrm{i}\theta})\}. \tag{3.12}$$

Proof. First we observe that $\widetilde{D}_4(1)=0$ by (3.11). Thus, taking $\theta\to 0$, we see that it suffices to prove the equality of the derivatives of both sides of (3.12). Since

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\,\mathrm{Ls}_4(\theta) = -\log^3\Big|2\sin\frac{\theta}{2}\Big| = -A^3,$$

by Corollary 3.2, we have

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\Big\{\frac{2}{3}\,\mathrm{Ls}_4(\theta)-\zeta(3)\theta+\widetilde{D}_4(e^{\mathrm{i}\theta})+4\widetilde{D}_4(1-e^{\mathrm{i}\theta})\Big\} = -\zeta(3)+\frac{\mathrm{Li}_3(e^{\mathrm{i}\theta})+\mathrm{Li}_3(e^{-\mathrm{i}\theta})}{2}+2\widetilde{D}_3(1-e^{\mathrm{i}\theta}). \tag{3.13}$$

Since $\mathrm{Li}_3(1)=\zeta(3)$ and $\lim_{\theta\to 0}\widetilde{D}_3(1-e^{\mathrm{i}\theta})=0$ by (3.8), it suffices to prove the derivative of (3.13) vanishes. Clearly, $\widetilde{D}_m(x)=D_m(x)$ for all even m by (3.7). Thus, using Corollary 3.2 again, we see that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}(\text{RHS of (3.13)}) = -\frac{\mathrm{Li}_2(e^{\mathrm{i}\theta})-\mathrm{Li}_2(e^{-\mathrm{i}\theta})}{2i} - \widetilde{D}_2(1-e^{\mathrm{i}\theta})$$
$$= -\widetilde{D}_2(e^{\mathrm{i}\theta})-\widetilde{D}_2(1-e^{\mathrm{i}\theta}) = -D_2(e^{\mathrm{i}\theta})-D_2(1-e^{\mathrm{i}\theta}) = 0 \tag{3.14}$$

by [16, equation (4)]. This completes the proof of Lemma 3.3. □

Lemma 3.4. *The following expression for* $\mathrm{Lsc}_{3,2}(\theta)$ *holds for all* $\theta\in(0,\pi)$*:*

$$\mathrm{Lsc}_{3,2}(\theta) = -\frac{\zeta(3)}{4}\theta - \frac{1}{2}\widetilde{D}_4(-e^{\mathrm{i}\theta}) - \widetilde{D}_4(e^{\mathrm{i}\theta}) + 2\widetilde{D}_4(1+e^{\mathrm{i}\theta}) + 2\widetilde{D}_4\Big(\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big) - \frac{1}{2}\widetilde{D}_4(1-e^{2\mathrm{i}\theta}). \tag{3.15}$$

Proof. The proof of this lemma is completely similar to that of Lemma 3.3. As above, let $A=A(\theta)$ and $B=B(\theta)$. By straightforward computations using Corollary 3.2, we find that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\,\mathrm{Lsc}_{3,2}(\theta) = -\log^2\Big|2\sin\frac{\theta}{2}\Big|\log\Big|2\cos\frac{\theta}{2}\Big| = -A^2B,$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_4(\pm e^{\mathrm{i}\theta}) = \widetilde{D}_3(\pm e^{\mathrm{i}\theta}) \xrightarrow{\mathrm{d}/\mathrm{d}\theta} -\widetilde{D}_2(\pm e^{\mathrm{i}\theta}),$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_4(1+e^{\mathrm{i}\theta}) = \frac{1}{2}\widetilde{D}_3(1+e^{\mathrm{i}\theta}) + \frac{B^3}{6} \xrightarrow{\mathrm{d}/\mathrm{d}\theta} -\frac{1}{4}\widetilde{D}_2(1+e^{\mathrm{i}\theta}) - \frac{1}{4}B^2a_1^+,$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_4\Big(\frac{1}{1+e^{\mathrm{i}\theta}}\Big) = -\frac{B^3}{12} - \frac{1}{2}\sum_{j=1}^{3}\frac{B^{3-j}}{(3-j)!}\Big(\frac{\mathrm{Li}_j(\frac{1}{1+e^{\mathrm{i}\theta}})}{1+e^{\mathrm{i}\theta}} + \frac{\mathrm{Li}_j(\frac{1}{1+e^{-\mathrm{i}\theta}})}{1+e^{-\mathrm{i}\theta}}\Big)$$

(which is used to compute the limit as $\theta\to 0$),

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_4\Big(\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big) = \frac{(B-A)^3}{12} \xrightarrow{\mathrm{d}/\mathrm{d}\theta} \frac{(A-B)^2(a_1^+-a_1^-)}{8},$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\widetilde{D}_4(1-e^{2\mathrm{i}\theta}) = \widetilde{D}_3(1-e^{2\mathrm{i}\theta}) + \frac{(A+B)^3}{3} \xrightarrow{\mathrm{d}/\mathrm{d}\theta} -\widetilde{D}_2(1-e^{2\mathrm{i}\theta}) - \frac{1}{2}(A+B)^2(a_1^++a_1^-).$$

Thus, by taking $\theta \to 0$, we see that the difference between the left-hand and right-hand sides of $\frac{\mathrm{d}}{\mathrm{d}\theta}$(RHS of (3.15)) is

$$\frac{\log^3(2)}{6} + \frac{5\zeta(3)}{4} + \frac{1}{2}\operatorname{Li}_3(-1) - \sum_{j=1}^{3} \frac{\log^{3-j}(2)}{(3-j)!}\operatorname{Li}_j\Big(\frac{1}{2}\Big) = 0$$

by the identities (see [10, (1.16), (6.5) and (6.12)])

$$\operatorname{Li}_2\Big(\frac{1}{2}\Big) = \frac{1}{2}(\zeta(2) - \log^2(2)), \quad \operatorname{Li}_3(-1) = -\frac{3}{4}\zeta(3), \quad \operatorname{Li}_3\Big(\frac{1}{2}\Big) = \frac{7}{8}\zeta(3) - \frac{1}{12}\pi^2\log(2) + \frac{1}{6}\log^3(2).$$

Thus we only need to show the second derivatives of both sides of (3.15) agree:

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\Big(-2A^2B + \frac{\mathrm{d}}{\mathrm{d}\theta}\Big\{2\widetilde{D}_4(e^{\mathrm{i}\theta}) + \widetilde{D}_4(-e^{\mathrm{i}\theta}) - 4\widetilde{D}_4(1+e^{\mathrm{i}\theta}) + \widetilde{D}_4(1-e^{2\mathrm{i}\theta}) - 4\widetilde{D}_4\Big(\frac{1-e^{\mathrm{i}\theta}}{1+e^{\mathrm{i}\theta}}\Big)\Big\}\Big) \stackrel{?}{=} 0. \tag{3.16}$$

Now we have

$$\begin{aligned}
\text{LHS of (3.16)} &= \frac{\mathrm{d}}{\mathrm{d}\theta}\Big(-2A^2B + 2\widetilde{D}_3(e^{\mathrm{i}\theta}) + \widetilde{D}_3(-e^{\mathrm{i}\theta}) - 4\Big(\frac{1}{2}\widetilde{D}_3(1+e^{\mathrm{i}\theta}) + \frac{B^3}{6}\Big) \\
&\qquad + \widetilde{D}_3(1-e^{2\mathrm{i}\theta}) + \frac{(A+B)^3}{3} - \frac{(A-B)^3}{3}\Big) \\
&= A^2a_1^+ + 2ABa_1^- - \widetilde{D}_2(-e^{\mathrm{i}\theta}) - 2\widetilde{D}_2(e^{\mathrm{i}\theta}) + \widetilde{D}_2(1+e^{\mathrm{i}\theta}) + B^2a_1^+ \\
&\qquad - \widetilde{D}_2(1-e^{2\mathrm{i}\theta}) - \frac{1}{2}(A+B)^2(a_1^+ + a_1^-) - \frac{1}{2}(A-B)^2(a_1^+ - a_1^-) \\
&= \widetilde{D}_2(e^{2\mathrm{i}\theta}) - 2\widetilde{D}_2(-e^{\mathrm{i}\theta}) - 2\widetilde{D}_2(e^{\mathrm{i}\theta}) = 0
\end{aligned}$$

by (3.14) and the distribution relation. This completes the proof of the lemma. □

Step 4. We will need the following functional equation of $\widetilde{D}_4$, which is a variant of Kummer's Li_4 equation [10, equation (7.78)]. (Note $\Lambda_4(x)$ therein is closely related to $\operatorname{Li}_4(-x)$; in particular, it only differs by products of lower weight terms. In order to convert from [10, equation (7.78)] to the $\widetilde{D}_4$ functional equation, we essentially only need to add a negative sign to all the arguments from [10, equation (7.78)] and drop any product terms.)

Let $\mathbb{Q}[\mathbb{CP}^1]$ be the set of finite $\mathbb{Q}$-linear combinations $\sum c_j[x_j]$ with $c_j \in \mathbb{Q}$, $x_j \in \mathbb{CP}^1$. We can then linearly extend $\widetilde{D}_m$ over $\mathbb{Q}[\mathbb{CP}^1]$.

Lemma 3.5 (Kummer). *For any $x, y \in \mathbb{C} \setminus \{0,1\}$, set $\xi = \xi_x := 1 - x$, $\eta = \eta_y := 1 - y$ and*

$$\begin{aligned}
H(x,y) := {}& \Big[\frac{x^2y}{\eta^2\xi}\Big] + \Big[-\frac{\eta x^2 y}{\xi}\Big] - 3\Big[-\frac{x}{\eta\xi}\Big] - 3\Big[-\frac{\eta x}{\xi}\Big] - 3\Big[\frac{x}{\eta}\Big] - 3[\eta x] \\
& + 6\Big[-\frac{x}{\xi}\Big] - 6\Big[-\frac{xy}{\eta}\Big] + 6[x] - 3\Big[\frac{xy}{\eta\xi}\Big] - 3[xy].
\end{aligned}$$

Then $F(x,y) := H(x,y) + H(y,x)$ is mapped to 0 under $\widetilde{D}_4$.

Proof. In order to verify that $\widetilde{D}_4(F(x,y)) = 0$ for all x, y, we apply [16, Proposition 1], which states that if $\{n_i, x_i(t)\}$ is a collection of integers n_i and rational functions of one variable $x_i(t)$, satisfying

$$\sum_i n_i[x_i(t)]^{m-2} \otimes ([x_i(t)] \wedge [1 - x_i(t)]) = 0, \tag{3.17}$$

in $\operatorname{Sym}^{m-2}(\mathbb{C}(t)^\times) \otimes \wedge^2(\mathbb{C}(t)^\times) \otimes_{\mathbb{Z}} \mathbb{Q}$, then $\sum_i n_i\widetilde{D}_m(x_i(t)) =$ constant. In this tensor condition, the tensors are multiplicative $(ab) \otimes c = a \otimes c + b \otimes c$, and we can ignore torsion (multiplication by roots of unity) in each slot. This tensor condition is closely related to the $\otimes^m$-invariant ("symbol") of multiple polylogarithms [8] and amounts to a convenient reformulation of the derivative of $\widetilde{D}_m(x_i(t))$ for the purposes of calculation.

Set $m = 4$, and fix $y = y_0 \in \mathbb{C}$. It is then straightforward (if tedious) to check that (3.17) vanishes for the list of coefficients and arguments in $F(x, y_0)$. Hence, for any fixed $y = y_0$, the combination $\widetilde{D}_4(F(x, y_0))$ is constant. By the symmetry of $F(x,y)$ with respect to $x \leftrightarrow y$, we also have by the same calculation that, for any fixed $x = x_0$, the combination $\widetilde{D}_4(F(x_0, y))$ is constant. It follows that $\widetilde{D}_4(F(x_1,y_1)) = \widetilde{D}_4(F(x_2,y_1)) = \widetilde{D}_4(F(x_2,y_2))$ for any $(x_1,y_1), (x_2,y_2) \in \mathbb{C}^2$, so $\widetilde{D}_4(F(x,y))$ is constant overall. Since $\widetilde{D}_4$ vanishes on the real line, and by specializing for example $x = y = \frac{1}{2}$ all arguments in $F(x,y)$ are real, this constant is necessarily 0. We have therefore established the required functional equation. □

Step 5. Specialization to the 12-th roots of unity. In the rest of this section, we put

$$\rho := e^{2\pi i/12}.$$

Note that, by applying (3.9) and (3.10) at most twice, we can make the argument of $\widetilde{D}_4$ lie in the upper half unit disk. We will often apply this rule in our calculations below.

By Lemma 3.3, we have

$$\mathrm{Ls}_4\Big(\frac{\pi}{3}\Big) = \frac{1}{2}\pi\zeta(3) + \frac{9}{2}\widetilde{D}_4(\rho^2). \tag{3.18}$$

We remark that in [4, equation (83c)], J. M. Borwein and A. Straub proved that $\mathrm{Ls}_4(\pi/3) = \pi\zeta(3)/2 + 9\,\mathrm{Cl}_4(\pi/3)/2$ (here Cl_4 is the Clausen function), which agrees with (3.18) because $\widetilde{D}_4(\rho^2) = \mathrm{Im}\,\mathrm{Li}_4(\rho^2) = \mathrm{Cl}_4(\pi/3)$.

By Lemma 3.4, we have

$$\mathrm{Lsc}_{3,2}\Big(\frac{\pi}{3}\Big) = -\frac{1}{12}\pi\zeta(3) - \widetilde{D}_4(\rho^2) + \frac{1}{2}\widetilde{D}_4(\rho^4) + \frac{5}{2}\widetilde{D}_4\Big(\frac{\rho}{\sqrt{3}}\Big) - 2\widetilde{D}_4\Big(\frac{\rho^3}{\sqrt{3}}\Big). \tag{3.19}$$

By Lemma 3.5, we have that $\widetilde{D}_4$ vanishes on $F(\rho^2, \rho^4)$, which implies

$$-9\widetilde{D}_4(\rho^2) + 6\widetilde{D}_4(\rho^4) - 15\widetilde{D}_4\Big(\frac{\rho}{\sqrt{3}}\Big) + 12\widetilde{D}_4\Big(\frac{\rho^3}{\sqrt{3}}\Big) = 0. \tag{3.20}$$

Note the distribution relation $\widetilde{D}_4(\rho^4) = 8\widetilde{D}_4(\rho^2) + 8\widetilde{D}_4(-\rho^2) = 8\widetilde{D}_4(\rho^2) - 8\widetilde{D}_4(\rho^4)$ implies that

$$\widetilde{D}_4(\rho^4) = \frac{8}{9}\widetilde{D}_4(\rho^2). \tag{3.21}$$

Combining (3.19), (3.20) and (3.21), we obtain

$$\mathrm{Lsc}_{3,2}\Big(\frac{\pi}{3}\Big) = -\frac{1}{12}\pi\zeta(3) - \frac{7}{6}\widetilde{D}_4(\rho^2). \tag{3.22}$$

Write $\rho^{1/2} := e^{2\pi i/24}$ and

$$r := |1-\rho| = \frac{\sqrt{6}-\sqrt{2}}{2}.$$

By Lemma 3.3 and Lemma 3.4, we have

$$\mathrm{Ls}_4\Big(\frac{5\pi}{6}\Big) = \frac{5}{4}\pi\zeta(3) - \frac{3}{2}\widetilde{D}_4(\rho^5) + 6\widetilde{D}_4(r\rho^{1/2}), \tag{3.23}$$

$$\mathrm{Lsc}_{3,2}\Big(\frac{\pi}{6}\Big) = -\frac{1}{24}\pi\zeta(3) - \widetilde{D}_4(\rho) + \frac{1}{2}\widetilde{D}_4(\rho^2) + \frac{1}{2}\widetilde{D}_4(\rho^5) + 2\widetilde{D}_4(r\rho^{1/2}) - 2\widetilde{D}_4(r^2\rho^3), \tag{3.24}$$

$$\mathrm{Lsc}_{3,2}\Big(\frac{5\pi}{6}\Big) = -\frac{5}{24}\pi\zeta(3) + \frac{1}{2}\widetilde{D}_4(\rho) - \frac{1}{2}\widetilde{D}_4(\rho^2) - \widetilde{D}_4(\rho^5) + 2\widetilde{D}_4(r\rho^{5/2}) - 2\widetilde{D}_4(r^2\rho^3). \tag{3.25}$$

By substituting first (3.1), (3.5), then (3.18), (3.22), (3.23), (3.24) and (3.25), the left-hand side of (1.1) is transformed as follows:

$$\begin{aligned}
&41\sum_{n=0}^{\infty}\frac{\binom{2n}{n}}{(2n+1)^4 16^n} + 9\sum_{n=1}^{\infty}\frac{\binom{2n}{n}H_{2n}}{(2n+1)^3 16^n}\\
&\quad= \frac{41}{6}\,\mathrm{Ls}_4\Big(\frac{\pi}{3}\Big) + 9\,\mathrm{Lsc}_{3,2}\Big(\frac{\pi}{3}\Big) + 18\,\mathrm{Ls}_4\Big(\frac{5\pi}{6}\Big) - 18\,\mathrm{Lsc}_{3,2}\Big(\frac{\pi}{6}\Big) + 36\,\mathrm{Lsc}_{3,2}\Big(\frac{5\pi}{6}\Big) - 18\pi\zeta(3)\\
&\quad= \frac{5}{12}\pi\zeta(3) + 36\widetilde{D}_4(\rho) - \frac{27}{4}\widetilde{D}_4(\rho^2) - 72\widetilde{D}_4(\rho^5) + 72\widetilde{D}_4(r\rho^{1/2}) + 72\widetilde{D}_4(r\rho^{5/2}) - 36\widetilde{D}_4(r^2\rho^3).
\end{aligned}$$

Since $\beta(4) = \mathrm{Im}(\mathrm{Li}_4(i)) = \widetilde{D}_4(\rho^3)$, the conjectured formula in (1.1) is reduced to

$$\widetilde{D}_4(\rho) - \frac{3}{16}\widetilde{D}_4(\rho^2) - \frac{10}{9}\widetilde{D}_4(\rho^3) - 2\widetilde{D}_4(\rho^5) + 2\widetilde{D}_4(r\rho^{1/2}) + 2\widetilde{D}_4(r\rho^{5/2}) - \widetilde{D}_4(r^2\rho^3) \stackrel{?}{=} 0. \tag{3.26}$$

By the distribution relation

$$\widetilde{D}_4(r^2\rho^3) = 8\widetilde{D}_4(r\rho^{3/2}) + 8\widetilde{D}_4(-r\rho^{3/2}) = 8\widetilde{D}_4(r\rho^{3/2}) - 8\widetilde{D}_4(r\rho^{9/2}),$$

it remains to show that

$$2\widetilde{D}_4(r\rho^{1/2}) - 8\widetilde{D}_4(r\rho^{3/2}) + 2\widetilde{D}_4(r\rho^{5/2}) + 8\widetilde{D}_4(r\rho^{9/2}) \overset{?}{=} -\widetilde{D}_4(\rho) + \frac{3}{16}\widetilde{D}_4(\rho^2) + \frac{10}{9}\widetilde{D}_4(\rho^3) + 2\widetilde{D}_4(\rho^5). \tag{3.27}$$

By specializing Lemma 3.5 to various choices of x, y, we obtain further relations between $\widetilde{D}_4$. In particular, since $\widetilde{D}_4$ vanishes on both $\frac{1}{3}F(\rho^2, \rho)$ and $\frac{1}{3}F(\rho^2, \rho^5)$, we have respectively

$$5\widetilde{D}_4(\rho) - 3\widetilde{D}_4(\rho^3) + 3\widetilde{D}_4(r\rho^{1/2}) - \widetilde{D}_4(r\rho^{3/2}) - 2\widetilde{D}_4(r\rho^{5/2}) + 3\widetilde{D}_4(r\rho^{9/2}) = 0, \tag{3.28}$$
$$-3\widetilde{D}_4(\rho^3) + 5\widetilde{D}_4(\rho^5) - 2\widetilde{D}_4(r\rho^{1/2}) - 3\widetilde{D}_4(r\rho^{3/2}) + 3\widetilde{D}_4(r\rho^{5/2}) + \widetilde{D}_4(r\rho^{9/2}) = 0. \tag{3.29}$$

By adding (3.28) and (3.29), we have

$$\widetilde{D}_4(r\rho^{1/2}) - 4\widetilde{D}_4(r\rho^{3/2}) + \widetilde{D}_4(r\rho^{5/2}) + 4\widetilde{D}_4(r\rho^{9/2}) = -5\widetilde{D}_4(\rho) + 6\widetilde{D}_4(\rho^3) - 5\widetilde{D}_4(\rho^5).$$

Therefore, (3.27) is reduced to

$$-9\widetilde{D}_4(\rho) - \frac{3}{16}\widetilde{D}_4(\rho^2) + \frac{98}{9}\widetilde{D}_4(\rho^3) - 12\widetilde{D}_4(\rho^5) \overset{?}{=} 0. \tag{3.30}$$

By the distribution relations, we have

$$\widetilde{D}_4(\rho^2) = 8\widetilde{D}_4(\rho) + 8\widetilde{D}_4(-\rho) \implies \widetilde{D}_4(\rho^2) = 8\widetilde{D}_4(\rho) - 8\widetilde{D}_4(\rho^5), \tag{3.31}$$
$$\widetilde{D}_4(\rho^3) = 27\widetilde{D}_4(\rho) + 27\widetilde{D}_4(\rho^5) + 27\widetilde{D}_4(\rho^9) \implies \widetilde{D}_4(\rho^3) = \frac{27}{28}\widetilde{D}_4(\rho) + \frac{27}{28}\widetilde{D}_4(\rho^5). \tag{3.32}$$

Equations (3.31) and (3.32) establish (3.30). Therefore, the proof of (1.1) is complete.

4 Proof of (1.2)

Let

$$\phi = \frac{\sqrt{5}+1}{2}$$

be the golden ratio. Setting $p = 2$ and $z = \frac{1}{4}$ in (2.3) and (2.5), we have $\theta = \log\phi$ and

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{(2n+1)^3(-16)^n} = -\frac{1}{2}\operatorname{Lsh}_3(2\log\phi), \tag{4.1}$$
$$\sum_{n=1}^{\infty} \frac{\binom{2n}{n}H_{2n}}{(2n+1)^2(-16)^n} = -2\operatorname{Lshch}_{2,2}(2\log\phi) + 4\operatorname{Lshch}_{1,3}(\log\phi) + 4\operatorname{Lshch}_{2,2}(\log\phi). \tag{4.2}$$

Lemma 4.1. *The following expressions for* $\operatorname{Lsh}_3(x)$, $\operatorname{Lshch}_{1,3}(x)$ *and* $\operatorname{Lshch}_{2,2}(x)$ *hold for all* $x \in (0, +\infty)$*:*

$$\operatorname{Lsh}_3(x) = -\widetilde{D}_3(e^{-x}) - 2\widetilde{D}_3(1-e^{-x}) - \frac{1}{3}x\log^2\Big(2\sinh\frac{x}{2}\Big) + \widetilde{D}_3(1), \tag{4.3}$$
$$\operatorname{Lshch}_{1,3}(x) = -\widetilde{D}_3(-e^{-x}) - 2\widetilde{D}_3\Big(\frac{1}{1+e^{-x}}\Big) - \frac{1}{3}x\log^2\Big(2\cosh\frac{x}{2}\Big) + \widetilde{D}_3(1), \tag{4.4}$$
$$\begin{aligned}\operatorname{Lshch}_{2,2}(x) = &-\frac{1}{8}\widetilde{D}_3(e^{-2x}) - \frac{1}{2}\widetilde{D}_3(1-e^{-2x}) + \widetilde{D}_3(1-e^{-x}) + \widetilde{D}_3\Big(\frac{1}{1+e^{-x}}\Big)\\ &- \frac{1}{3}x\log\Big(2\sinh\frac{x}{2}\Big)\log\Big(2\cosh\frac{x}{2}\Big) - \frac{3}{4}\widetilde{D}_3(1).\end{aligned} \tag{4.5}$$

Remark 4.2. Using the shorthand $\psi(t) := \widetilde{D}_3(1-t) - \widetilde{D}_3(1-1/t)$ and adding suitable 3-term relations for $\widetilde{D}_3$, Lemma 4.1 can be stated more succinctly and uniformly as follows:

$$\operatorname{Lshch}_{j,k}(x) + \frac{x}{3}\log^{j-1}\Big(2\sinh\Big(\frac{x}{2}\Big)\Big)\log^{k-1}\Big(2\cosh\Big(\frac{x}{2}\Big)\Big) = \begin{cases}\psi(e^x) & \text{for } (j,k) = (3,1),\\ \frac{1}{4}(\psi(e^{2x}) - 2\psi(e^x) - 2\psi(e^{-x})) & \text{for } (j,k) = (2,2),\\ \psi(-e^x) & \text{for } (j,k) = (1,3).\end{cases}$$

Proof. Suppose $x \in (0, +\infty)$. Let $f_1(x)$ be the difference between the left-hand and right-hand sides of (4.3). Clearly, $\lim_{x\to 0} f_1(x) = 0$. By the definitions of $\widetilde{D}_3$ and Lsh_3, and the simple identity

$$\log\Big(2\sinh\Big(\frac{x}{2}\Big)\Big) = \frac{x}{2} + \log(1-e^{-x}),$$

we may rewrite $f_1(x)$ as

$$\begin{aligned} f_1(x) = -\int_0^x \Big(\frac{t}{2} + \log(1-e^{-t})\Big)^2 \mathrm{d}t + \mathrm{Li}_3(e^{-x}) + x\,\mathrm{Li}_2(e^{-x}) + 2\,\mathrm{Li}_3(1-e^{-x}) \\ - 2\log(1-e^{-x})\,\mathrm{Li}_2(1-e^{-x}) + x\log^2(1-e^{-x}) + \frac{1}{12}x^3 - \zeta(3). \end{aligned}$$

Then a straightforward computation gives $f_1'(x) = 0$, which completes the proof of (4.3).

Let $f_2(x)$ be the difference between the left-hand and right-hand sides of (4.4). We have

$$\lim_{x\to 0} f_2(x) = \widetilde{D}_3(-1) + 2\widetilde{D}_3\Big(\frac{1}{2}\Big) - \widetilde{D}_3(1) = 0$$

by the following identities:

$$\widetilde{D}_3(-1) = -\frac{3}{4}\widetilde{D}_3(1) \quad \text{and} \quad \widetilde{D}_3\Big(\frac{1}{2}\Big) = \frac{7}{8}\widetilde{D}_3(1). \tag{4.6}$$

(The first identity in (4.6) follows from the duplication relation $\widetilde{D}_3(1) = 4\widetilde{D}_3(1) + 4\widetilde{D}_3(-1)$. See [10, (6.12) and (1.16)] for the second.)

By the definitions of $\widetilde{D}_3$ and $\mathrm{Lshch}_{1,3}$, and the identity $\log(2\cosh(\frac{x}{2})) = \frac{x}{2} + \log(1+e^{-x})$, we may rewrite $f_2(x)$ as

$$\begin{aligned} f_2(x) = -\int_0^x \Big(\frac{t}{2} + \log(1+e^{-t})\Big)^2 \mathrm{d}t + \mathrm{Li}_3(-e^{-x}) + x\,\mathrm{Li}_2(-e^{-x}) + 2\,\mathrm{Li}_3\Big(\frac{1}{1+e^{-x}}\Big) \\ + 2\log(1+e^{-x})\,\mathrm{Li}_2\Big(\frac{1}{1+e^{-x}}\Big) + \frac{2}{3}\log^3(1+e^{-x}) + x\log^2(1+e^{-x}) + \frac{1}{12}x^3 - \zeta(3). \end{aligned}$$

Then a straightforward computation gives $f_2'(x) = 0$, which completes the proof of (4.4).

Observing that $\log(2\sinh x) = \log(2\sinh(\frac{x}{2})) + \log(2\cosh(\frac{x}{2}))$, we have

$$\begin{aligned} \mathrm{Lsh}_3(2x) = -2\int_0^x \log^2(\sinh t)\,\mathrm{d}t = -2\int_0^x \Big(\log\Big(\sinh\frac{t}{2}\Big) + \log\Big(\cosh\frac{t}{2}\Big)\Big)^2 \mathrm{d}t \\ = 2\,\mathrm{Lsh}_3(x) + 4\,\mathrm{Lshch}_{2,2}(x) + 2\,\mathrm{Lshch}_{1,3}(x). \end{aligned}$$

Therefore,

$$\mathrm{Lshch}_{2,2}(x) = \frac{1}{4}\,\mathrm{Lsh}_3(2x) - \frac{1}{2}\,\mathrm{Lsh}_3(x) - \frac{1}{2}\,\mathrm{Lshch}_{1,3}(x). \tag{4.7}$$

Equation (4.5) follows immediately by substituting (4.3) and (4.4) into (4.7), and using the duplication relation $\widetilde{D}_3(e^{-2x}) = 4\widetilde{D}_3(e^{-x}) + 4\widetilde{D}_3(-e^{-x})$. □

Specializing Lemma 4.1 at $x = \log\phi$ and $x = 2\log\phi$ and simplifying the golden ratio combinations via

$$1-\phi^{-2} = \phi^{-1}, \quad 1+\phi^{-2} = \sqrt{5}\phi^{-1}, \quad 1-\phi^{-4} = \sqrt{5}\phi^{-2},$$

we directly find

$$\begin{aligned} \mathrm{Lsh}_3(2\log\phi) &= -\widetilde{D}_3\Big(\frac{1}{\phi^2}\Big) - 2\widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \widetilde{D}_3(1), \\ \mathrm{Lshch}_{2,2}(2\log\phi) &= -\frac{1}{8}\widetilde{D}_3\Big(\frac{1}{\phi^4}\Big) - \frac{1}{2}\widetilde{D}_3\Big(\frac{\sqrt{5}}{\phi^2}\Big) + \widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \widetilde{D}_3\Big(\frac{\phi}{\sqrt{5}}\Big) - \frac{3}{4}\widetilde{D}_3(1), \\ \mathrm{Lshch}_{1,3}(\log\phi) &= -\widetilde{D}_3\Big(-\frac{1}{\phi}\Big) - 2\widetilde{D}_3\Big(\frac{1}{\phi}\Big) - \frac{3}{4}\log^3\phi + \widetilde{D}_3(1), \\ \mathrm{Lshch}_{2,2}(\log\phi) &= \frac{7}{8}\widetilde{D}_3\Big(\frac{1}{\phi^2}\Big) + \frac{1}{2}\widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \frac{3}{4}\log^3\phi - \frac{3}{4}\widetilde{D}_3(1). \end{aligned}$$

Then, by substituting the duplication relation

$$\widetilde{D}_3\Big(-\frac{1}{\phi}\Big) = -\widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \frac{1}{4}\widetilde{D}_3\Big(\frac{1}{\phi^2}\Big)$$

and the following evaluation of $\widetilde{D}_3(\phi^{-2})$ (see [10, (6.13) and (1.20)]):

$$\widetilde{D}_3\Big(\frac{1}{\phi^2}\Big) = \frac{4}{5}\widetilde{D}_3(1),$$

into the above equations, we obtain

$$\mathrm{Lsh}_3(2\log\phi) = -2\widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \frac{1}{5}\widetilde{D}_3(1), \tag{4.8}$$

$$\mathrm{Lshch}_{2,2}(2\log\phi) = -\frac{1}{8}\widetilde{D}_3\Big(\frac{1}{\phi^4}\Big) - \frac{1}{2}\widetilde{D}_3\Big(\frac{\sqrt{5}}{\phi^2}\Big) + \widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \widetilde{D}_3\Big(\frac{\phi}{\sqrt{5}}\Big) - \frac{3}{4}\widetilde{D}_3(1), \tag{4.9}$$

$$\mathrm{Lshch}_{1,3}(\log\phi) = -\widetilde{D}_3\Big(\frac{1}{\phi}\Big) - \frac{3}{4}\log^3\phi + \frac{4}{5}\widetilde{D}_3(1), \tag{4.10}$$

$$\mathrm{Lshch}_{2,2}(\log\phi) = \frac{1}{2}\widetilde{D}_3\Big(\frac{1}{\phi}\Big) + \frac{3}{4}\log^3\phi - \frac{1}{20}\widetilde{D}_3(1). \tag{4.11}$$

By substituting first (4.1), (4.2), then (4.8)–(4.11), the left-hand side of (1.2) is transformed as follows:

$$\begin{aligned} 17\sum_{n=0}^{\infty}\frac{\binom{2n}{n}}{(2n+1)^3(-16)^n} + 5\sum_{n=1}^{\infty}\frac{\binom{2n}{n}H_{2n}}{(2n+1)^2(-16)^n} &= -\frac{17}{2}\,\mathrm{Lsh}_3(2\log\phi) - 10\,\mathrm{Lshch}_{2,2}(2\log\phi) + 20\,\mathrm{Lshch}_{1,3}(\log\phi) + 20\,\mathrm{Lshch}_{2,2}(\log\phi) \\ &= \frac{5}{4}\widetilde{D}_3\Big(\frac{1}{\phi^4}\Big) + 5\widetilde{D}_3\Big(\frac{\sqrt{5}}{\phi^2}\Big) - 3\widetilde{D}_3\Big(\frac{1}{\phi}\Big) - 10\widetilde{D}_3\Big(\frac{\phi}{\sqrt{5}}\Big) + \frac{104}{5}\widetilde{D}_3(1). \end{aligned}$$

Since $\widetilde{D}_3(1) = \zeta(3)$ and the right-hand side of (1.2) is $14\zeta(3)$, the conjectured identity (1.2) is equivalent to

$$\frac{5}{4}\widetilde{D}_3\Big(\frac{1}{\phi^4}\Big) + 5\widetilde{D}_3\Big(\frac{\sqrt{5}}{\phi^2}\Big) - 3\widetilde{D}_3\Big(\frac{1}{\phi}\Big) - 10\widetilde{D}_3\Big(\frac{\phi}{\sqrt{5}}\Big) + \frac{34}{5}\widetilde{D}_3(1) \overset{?}{=} 0. \tag{4.12}$$

We shall prove this by specializing a suitable $\widetilde{D}_3$ functional equation.

Lemma 4.3. *The following linear combination $G(x)$ vanishes identically under $\widetilde{D}_3$:*

$$\begin{aligned} G(x) := {} & 5\Big[\frac{1-2x}{(1-x)^3(1+x)}\Big] + 6\Big[-\frac{(1-x)^3}{(2-x)^3}\Big] - 6\Big[\frac{1}{(1-x)^3}\Big] - 15\Big[\frac{(1-x)(1+x)}{1-2x}\Big] - 15\Big[\frac{1-2x}{(1-x)^2}\Big] \\ & - 18\Big[\frac{1-x}{(2-x)^2}\Big] + 18\Big[-\frac{1}{(1-x)(2-x)}\Big] - 3\Big[\frac{1}{(1-x)(1+x)}\Big] - 10\Big[\frac{1-2x}{2-x}\Big] - 10\Big[\frac{2-x}{1+x}\Big] \\ & + 15\Big[-\frac{x}{1-2x}\Big] + 15\Big[\frac{x}{1-x}\Big] - 24\Big[-\frac{1-x}{1+x}\Big] + 24\Big[\frac{1-x}{1+x}\Big] + 45\Big[\frac{1-2x}{1-x}\Big] - 54\Big[-\frac{1-x}{2-x}\Big] \\ & + 36\Big[\frac{1}{2-x}\Big] + 6\Big[\frac{1}{1-x}\Big] - 18\Big[\frac{1}{1+x}\Big] + 42\Big[-\frac{1}{1-x}\Big] - 34\big[1\big]. \end{aligned}$$

Proof. The proof strategy is exactly the same as for Lemma 3.5; we apply the tensor criterion in (3.17) in the case $m = 3$. This shows that $\widetilde{D}_3(G(x))$ is constant. To fix the constant, we specialize to $x = 0$. We find (simplifying only with inversion at the moment) that

$$\widetilde{D}_3(G(0)) = 18\widetilde{D}_3(-1) - 36\widetilde{D}_3\Big(-\frac{1}{2}\Big) + 6\widetilde{D}_3\Big(-\frac{1}{8}\Big) + 30\widetilde{D}_3(0) - 18\widetilde{D}_3\Big(\frac{1}{4}\Big) + 16\widetilde{D}_3\Big(\frac{1}{2}\Big) - 11\widetilde{D}_3(1).$$

This time, using the duplication relation $\widetilde{D}_3(\frac{1}{4}) = 4\widetilde{D}_3(\frac{1}{2}) + 4\widetilde{D}_3(-\frac{1}{2})$ to eliminate $\widetilde{D}_3(\frac{1}{4})$ and simplifying with $\widetilde{D}_3(0) = 0$, we obtain

$$\widetilde{D}_3(G(0)) = 18\widetilde{D}_3(-1) - 108\widetilde{D}_3\Big(-\frac{1}{2}\Big) + 6\widetilde{D}_3\Big(-\frac{1}{8}\Big) - 56\widetilde{D}_3\Big(\frac{1}{2}\Big) - 11\widetilde{D}_3(1).$$

But we can show this vanishes by using (4.6) and the well-known identity (see [10, p. 179])

$$\widetilde{D}_3\Big(-\frac{1}{8}\Big) - 18\widetilde{D}_3\Big(-\frac{1}{2}\Big) = \frac{49}{4}\widetilde{D}_3(1).$$

With this, the functional equation in the lemma is now proven. □

Now consider $\widetilde{D}_3(G(-\phi^{-1}))$. We first put all real arguments into the interval $[0,1]$ by applying the duplication relation and inversion relation

$$\widetilde{D}_3(x^2) = 4(\widetilde{D}(x) + \widetilde{D}(-x)), \quad \widetilde{D}_3(x^{-1}) = \widetilde{D}_3(x).$$

Then we obtain exactly

$$0 = \widetilde{D}_3(G(-\phi^{-1})) = -\frac{25}{4}\widetilde{D}_3\Big(\frac{1}{\phi^4}\Big) - 25\widetilde{D}_3\Big(\frac{\sqrt{5}}{\phi^2}\Big) + 15\widetilde{D}_3\Big(\frac{1}{\phi}\Big) + 50\widetilde{D}_3\Big(\frac{\phi}{\sqrt{5}}\Big) - 34\widetilde{D}_3(1).$$

This is -5 times the left-hand side of (4.12); hence the left-hand side of (4.12) is equal to exactly 0. The proof of (1.2) is complete.

Remark 4.4. It should be noted that the functional equation in Lemma 4.3 has been concocted to give a simple proof of (4.12) in the previous lines. This functional equation can be broken down into a number of smaller functional equations, with slightly more structured coefficients. Specifically, Lemma 4.3 is a combination of the following four linearly independent functional equations (irreducible within the selected set of arguments):

$$\begin{aligned}
&\widetilde{D}_3\Big(-\Big[\frac{1-2x}{(1-x)^3(1+x)}\Big] + 3\Big[\frac{1-2x}{(1-x)^2}\Big] + 3\Big[\frac{(1-x)(1+x)}{1-2x}\Big] + 3\Big[\frac{1}{(1-x)(1+x)}\Big]\\
&\qquad - 6\Big[\frac{1-2x}{1-x}\Big] + 2\Big[\frac{1-2x}{2-x}\Big] + 2\Big[\frac{2-x}{1+x}\Big] + 6\Big[-\frac{1}{1-x}\Big] - 6\Big[\frac{1}{1+x}\Big] + 5[1]\Big) = 0,\\
&\widetilde{D}_3\Big(-\Big[-\frac{(1-x)^3}{(2-x)^3}\Big] + \Big[\frac{1}{(1-x)^3}\Big] + 3\Big[\frac{1-x}{(2-x)^2}\Big] - 3\Big[-\frac{1}{(1-x)(2-x)}\Big] + 9\Big[-\frac{1-x}{2-x}\Big]\\
&\qquad - 12\Big[-\frac{1}{1-x}\Big] - 9\Big[\frac{1}{1-x}\Big] - 6\Big[\frac{1}{2-x}\Big] + 6[1]\Big) = 0,\\
&\widetilde{D}_3\Big(2\Big[\frac{1}{(1-x)(1+x)}\Big] - 4\Big[-\frac{1-x}{1+x}\Big] + 4\Big[\frac{1-x}{1+x}\Big] - 8\Big[\frac{1}{1-x}\Big] - 8\Big[\frac{1}{1+x}\Big] + 7[1]\Big) = 0,\\
&\widetilde{D}_3\Big(\Big[\frac{x}{1-x}\Big] + \Big[\frac{1-2x}{1-x}\Big] + \Big[-\frac{x}{1-2x}\Big] - [1]\Big) = 0.
\end{aligned} \tag{4.13}$$

Each of these can be proven in exactly the same way as Lemma 4.3 itself. In fact, the last one (4.13) is (up to inversion) a re-parameterization of the 3-term [10, equation (6.10)] functional equation

$$\widetilde{D}_3(x) + \widetilde{D}_3(1-x) + \widetilde{D}_3(1-x^{-1}) = \widetilde{D}_3(1), \quad \text{with } x \mapsto \frac{x}{1-x}.$$

Remark 4.5. We originally discovered the proof of (1.2) by expressing (4.1) and (4.2) in terms of colored multiple zeta values by applying Au's mechanism developed in [2]. Then (1.2) also follows from the computer-aided proof using Au's Mathematica package. For the detailed definition and introduction of colored multiple zeta values, see [17, Chapters 13–14].

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