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t-adic symmetric multiple zeta values for indices in which 1 and 3 appear alternately

by

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Abstract. This paper deals with the t-adic symmetric multiple zeta values modulo t^m without modulo π^2 reduction for indices in which 1 and 3 appear alternately. We investigate those values that can be expressed as a polynomial of the Riemann zeta values, and give a conjecturally complete list of explicit formulas for such values.

1. Introduction

1.1. Multiple zeta values and t-adic symmetric multiple zeta values. An *index* is a finite (possibly empty) sequence of positive integers. We say that an index is *admissible* if either it is empty or its last component is greater than 1.

For each admissible index $\boldsymbol{k} = (k_1, \dots, k_r)$, the *multiple zeta value* (*MZV*) is defined by

$$\zeta(\boldsymbol{k}) = \zeta(k_1, \dots, k_r) = \sum_{1 \le n_1 < \cdots < n_r} \frac{1}{n_1^{k_1} \cdots n_r^{k_r}} \in \mathbb{R},$$

where we set $\zeta(\emptyset) = 1$. Let $\mathcal{Z}$ denote the $\mathbb{Q}$-linear subspace of $\mathbb{R}$ spanned by all MZVs (including 1).

For each (not necessarily admissible) index $\boldsymbol{k}$, we write $\zeta^*(\boldsymbol{k})$ and $\zeta^{ш}(\boldsymbol{k})$ for the real numbers in $\mathcal{Z}$ obtained by taking the constant terms of the harmonic and shuffle regularizations, respectively (see [8] for details). Note that $\zeta^*(1) = \zeta^{ш}(1) = 0$ and that $\zeta^*(\boldsymbol{k}) = \zeta^{ш}(\boldsymbol{k}) = \zeta(\boldsymbol{k})$ if $\boldsymbol{k}$ is admissible.

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For each index $\boldsymbol{k} = (k_1, \dots, k_r)$, each symbol $\bullet \in \{*, ш\}$, and each non-negative integer m, we define

$$\zeta_m^\bullet(\boldsymbol{k}) = \sum_{\substack{l_1,\dots,l_r \geq 0 \\ l_1+\cdots+l_r=m}} \zeta^\bullet(k_1+l_1, \dots, k_r+l_r) \prod_{i=1}^{r} \binom{k_i+l_i-1}{l_i}.$$

Define the *t-adic symmetric multiple zeta value* (*t-adic SMZV*) by

$$\zeta_{\widehat{\mathcal{S}}}^\bullet(\boldsymbol{k}) = \sum_{i=0}^{r} (-1)^{k_{i+1}+\cdots+k_r} \zeta^\bullet(k_1, \dots, k_i) \sum_{m \geq 0} \zeta_m^\bullet(k_r, \dots, k_{i+1}) t^m \in \mathcal{Z}[[t]],$$

and define the *t-adic SMZV modulo* t^m by

$$\zeta_{\mathcal{S}_m}^\bullet(\boldsymbol{k}) = \pi_m(\zeta_{\widehat{\mathcal{S}}}^\bullet(\boldsymbol{k})) \in \mathcal{Z}[[t]]/(t^m)$$

for each positive integer m, where $\pi_m \colon \mathcal{Z}[[t]] \to \mathcal{Z}[[t]]/(t^m)$ is the natural projection. Here we set $\zeta_{\widehat{\mathcal{S}}}^\bullet(\emptyset) = 1$. The t-adic SMZVs have been studied in [9, 16, 14] as a generalization of ordinary SMZVs (the t-adic SMZVs for $t = 0$ or the t-adic SMZVs modulo t; see [10, 11]), in view of the Kaneko–Zagier conjecture concerning the t-adic SMZVs modulo t and the finite MZVs and of its generalization concerning the t-adic SMZVs and the $\boldsymbol{p}$-adic finite MZVs.

In this paper, we concentrate on indices $\boldsymbol{k}$ in which 1 and 3 appear alternately, such as (3), $(1, 3, 1)$, and $(3, 1, 3, 1)$. As a consequence, for all indices that appear in this paper, the values of ζ^* and $\zeta^ш$ coincide, and so do the values of $\zeta_{\widehat{\mathcal{S}}}^*$ and $\zeta_{\widehat{\mathcal{S}}}^ш$ (see Proposition 2.3); we therefore often omit $*$ and ш hereinafter.

Let $\boldsymbol{k}$ be an index in which 1 and 3 appear alternately. It is known that $\zeta(\boldsymbol{k})$ can be written as a polynomial of the Riemann zeta values (see [5, 6, 2, 1]). It turns out, however, that this is not always the case for $\zeta_{\widehat{\mathcal{S}}}(\boldsymbol{k})$. Our results, to be described in precise terms in the next subsection, explicitly write the value $\zeta_{\mathcal{S}_m}(\boldsymbol{k})$ as a polynomial of the Riemann zeta values for as large m as practically possible, in the light of the fact that almost no $\zeta_{\mathcal{S}_m}(\boldsymbol{k})$ with $m \geq 4$ is expected to be expressible as a polynomial of the Riemann zeta values.

We remark that our theorems and conjectures given in the next subsection concerning the t-adic SMZVs modulo π^2 are also likely to be valid for the $\boldsymbol{p}$-adic finite MZVs since the t-adic SMZVs modulo π^2 and the $\boldsymbol{p}$-adic finite MZVs are conjecturally isomorphic (for details, see [10, 11, 14]; see also [17, 12] for previous work on $\boldsymbol{p}$-adic finite MZVs).

1.2. Statements of our main theorems. We now give precise statements of our main theorems and conjectures. The proofs of the theorems will be given in the next section.

Let $\boldsymbol{k}$ be an index in which 1 and 3 appear alternately. According to its first and last components, we divide into the following four cases:

$$\boldsymbol{k} = (\{3,1\}^n, 3), (\{1,3\}^n), (\{3,1\}^n), (\{1,3\}^n, 1),$$

where n is a nonnegative integer and $\{a,b\}^n$ denotes the n-fold repetition of a, b, e.g., $\{a,b\}^2 = a,b,a,b$.

1.2.1. *Case of* $\boldsymbol{k} = (\{3,1\}^n, 3)$. Suppose that $\boldsymbol{k}$ both starts and ends with 3, i.e., $\boldsymbol{k}$ is of the form $(\{3,1\}^n, 3)$. Then we have $\zeta_{\mathcal{S}_1}(\boldsymbol{k}) = 0$ by definition. Since the coefficient of t in $\zeta_{\mathcal{S}_2}(3,1,3)$ is congruent to

$$-5\zeta(3)\zeta(5) - \zeta(3,5)$$

modulo π^2 (here and throughout, we have used [3] in numerical computations), it is reasonable to believe that $\zeta_{\mathcal{S}_2}(3,1,3)$ cannot be written as a polynomial of the Riemann zeta values even when reduced modulo π^2, and so we do not investigate $\zeta_{\mathcal{S}_m}(\{3,1\}^n, 3)$ for $m \geq 2$ in this paper.

1.2.2. *Case of* $\boldsymbol{k} = (\{1,3\}^n)$. Suppose that $\boldsymbol{k}$ starts with 1 and ends with 3, i.e., $\boldsymbol{k}$ is of the form $(\{1,3\}^n)$. Then we can compute $\zeta_{\mathcal{S}_2}(\boldsymbol{k})$ explicitly (recall that $\zeta(1) = 0$):

THEOREM 1.1. *We have*

$$\begin{aligned}\zeta_{\mathcal{S}_2}(\{1,3\}^n) = {}& \frac{2(-4)^n}{(4n+2)!}\pi^{4n} \\ &+ \Bigg(\sum_{\substack{n_0,n_1 \geq 0 \\ n_0+n_1=n}} \frac{(-4)^{n_0+1}(2-(-4)^{-n_1})}{(4n_0+2)!}\pi^{4n_0}\zeta(4n_1+1) \\ &\qquad - (-1)^n \sum_{\substack{n_0,n_1 \geq 0 \\ n_0+n_1=2n \\ n_0,n_1 \text{ odd}}} \frac{2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\Bigg)t\end{aligned}$$

for every nonnegative integer n.

Recall that Ono, Sakurada, and Seki [13, Theorem 4.1] computed the values of $\zeta_{\mathcal{S}_2}$ modulo π^2 for a wider class of indices. What makes Theorem 1.1 interesting is that it computes the values without modulo π^2 reduction.

Since the coefficient of t^2 in $\zeta_{\mathcal{S}_3}(1,3,1,3)$ is

$$\tfrac{1}{2}\zeta(2)\zeta(3)\zeta(5) + \zeta(2)\zeta(3,5) - \tfrac{1}{2}\zeta(3)^2\zeta(4) - \tfrac{1}{4}\zeta(3)\zeta(7) + \tfrac{81}{8}\zeta(5)^2 - \tfrac{103}{10}\zeta(10),$$

it is reasonable to believe that $\zeta_{\mathcal{S}_3}(1,3,1,3)$ cannot be written as a polynomial of the Riemann zeta values. Nevertheless, numerical experiments suggest that $\zeta_{\mathcal{S}_3}(\{1,3\}^n)$ modulo π^2 can always be written as a polynomial of the Riemann zeta values, and we make the following conjecture:

Conjecture 1.2. *We have*

$$\zeta_{\mathcal{S}_3}(\{1,3\}^n) \equiv \delta_{n,0} + (2(-4)^{-n} - 4)\zeta(4n+1)t + \Bigg(-2(-4)^{-n} \sum_{\substack{n_1,n_2\geq 0\\ n_1+n_2=n-1}} \zeta(4n_1+3)\zeta(4n_2+3) + 2\sum_{\substack{n_1,n_2\geq 0\\ n_1+n_2=n}} ((-4)^{-n_1}-2)((-4)^{-n_2}-2)\zeta(4n_1+1)\zeta(4n_2+1)\Bigg)t^2 \pmod{\pi^2}$$

for every nonnegative integer n, where $\delta_{n,0}$ denotes the Kronecker delta.

Since the coefficient of t^3 in $\zeta_{\mathcal{S}_4}(1,3,1,3)$ is congruent to

$$-\tfrac{845}{4}\zeta(11) - \tfrac{9}{4}\zeta(3)^2\zeta(5) - \zeta(3)\zeta(3,5) + 2\zeta(3,3,5)$$

modulo π^2, it is reasonable to believe that $\zeta_{\mathcal{S}_4}(1,3,1,3)$ cannot be written as a polynomial of the Riemann zeta values even when reduced modulo π^2, and so we do not investigate $\zeta_{\mathcal{S}_m}(\{1,3\}^n)$ for $m \geq 4$ in this paper.

1.2.3. *Case of $\boldsymbol{k} = (\{3,1\}^n)$.* Suppose that $\boldsymbol{k}$ starts with 3 and ends with 1, i.e., $\boldsymbol{k}$ is of the form $(\{3,1\}^n)$. Then we can compute $\zeta_{\mathcal{S}_3}(\boldsymbol{k})$ explicitly:

Theorem 1.3. *We have*

$$\zeta_{\mathcal{S}_3}(\{3,1\}^n) = \frac{2(-4)^n}{(4n+2)!}\pi^{4n} + (-1)^{n+1}\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n}} \frac{(-1)^{n_0}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)t + (-1)^n \sum_{\substack{n_0,n_1,n_2\geq 0\\ n_0+n_1+n_2=2n}} \frac{(-1)^{n_0}2^{n_0-n_1-n_2+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\zeta(2n_2+1)t^2$$

for every nonnegative integer n.

Corollary 1.4. *We have*

$$\zeta_{\mathcal{S}_3}(\{3,1\}^n) \equiv \delta_{n,0} - 2(-4)^{-n}\zeta(4n+1)t + 2(-4)^{-n}\sum_{\substack{n_1,n_2\geq 0\\ n_1+n_2=2n}} \zeta(2n_1+1)\zeta(2n_2+1)t^2 \pmod{\pi^2}$$

for every nonnegative integer n.

Since the coefficient of t^3 in $\zeta_{\mathcal{S}_4}(3,1,3,1)$ is congruent to

$$\tfrac{605}{4}\zeta(11) + \tfrac{19}{4}\zeta(3)^2\zeta(5) + 2\zeta(3)\zeta(3,5) - 2\zeta(3,3,5)$$

modulo π^2, it is reasonable to believe that $\zeta_{\mathcal{S}_4}(3,1,3,1)$ cannot be written as a polynomial of the Riemann zeta values even when reduced modulo π^2, and so we do not investigate $\zeta_{\mathcal{S}_m}(\{3,1\}^n)$ for $m \geq 4$ in this paper.

1.2.4. *Case of* $\boldsymbol{k} = (\{1,3\}^n, 1)$. Suppose that $\boldsymbol{k}$ both starts and ends with 1, i.e., $\boldsymbol{k}$ is of the form $(\{1,3\}^n, 1)$. Then we can compute $\zeta_{\mathcal{S}_3}(\boldsymbol{k})$ explicitly:

THEOREM 1.5. *We have*

$$\zeta_{\mathcal{S}_3}(\{1,3\}^n, 1) = \frac{(-4)^{n+1}}{(4n+4)!}\pi^{4n+2}t + (-1)^n \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n+1}} \frac{(-1)^{n_1}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)t^2$$

for every nonnegative integer n.

COROLLARY 1.6. *We have*

$$\zeta_{\mathcal{S}_3}(\{1,3\}^n, 1) \equiv -(-4)^{-n}\zeta(4n+3)t^2 \pmod{\pi^2}$$

for every nonnegative integer n.

Since the coefficient of t^3 in $\zeta_{\mathcal{S}_4}(1,3,1)$ is congruent to

$$\tfrac{9}{2}\zeta(3)\zeta(5) + \zeta(3,5)$$

modulo π^2, it is reasonable to believe that $\zeta_{\mathcal{S}_4}(1,3,1)$ cannot be written as a polynomial of the Riemann zeta values even when reduced modulo π^2, and so we do not investigate $\zeta_{\mathcal{S}_m}(\{1,3\}^n, 1)$ for $m \geq 4$ in this paper.

1.2.5. *Summary*

CONJECTURE 1.7. *The pairs* $(\boldsymbol{k}, m)$ *of an index* $\boldsymbol{k}$ *in which* 1 *and* 3 *appear alternately and a positive integer* m *such that* $\zeta_{\mathcal{S}_m}(\boldsymbol{k})$ *can be written as a polynomial of the Riemann zeta values are exhausted by those deduced from Theorems* 1.1, 1.3, *and* 1.5 *and the following equations:*

$$\zeta_{\mathcal{S}_1}(\{3,1\}^n, 3) = 0 \quad (n \geq 0),$$

$$\zeta_{\widehat{\mathcal{S}}}(1) = -\sum_{m\geq 1}\zeta(m+1)t^m,$$

$$\zeta_{\widehat{\mathcal{S}}}(3) = -\frac{1}{2}\sum_{m\geq 1}(m+1)(m+2)\zeta(m+3)t^m,$$

$$\zeta_{\mathcal{S}_3}(1,3) = -\frac{\pi^4}{90} + \left(\frac{\pi^2}{6}\zeta(3) - \frac{9}{2}\zeta(5)\right)t + \left(-\frac{19\pi^6}{3780} + \frac{1}{2}\zeta(3)^2\right)t^2 + \left(\frac{\pi^4}{90}\zeta(3) + \pi^2\zeta(5) - 17\zeta(7)\right)t^3,$$

$$\zeta_{\mathcal{S}_3}(3,1) = -\frac{\pi^4}{90} + \left(-\frac{\pi^2}{6}\zeta(3) + \frac{1}{2}\zeta(5)\right)t - \frac{1}{2}\zeta(3)^2t^2 + \left(\frac{\pi^4}{45}\zeta(3) - 3\zeta(7)\right)t^3.$$

2. Proofs of our main theorems

2.1. Algebraic setup. We use Hoffman's algebraic setup with a slightly different convention (see [7]). Set $\mathfrak{H} = \mathbb{Q}\langle x, y\rangle$, $\mathfrak{H}^1 = \mathbb{Q} + y\mathfrak{H}$, and $\mathfrak{H}^0 = \mathbb{Q} + y\mathfrak{H}x$. We define the *shuffle product* as the $\mathbb{Q}$-bilinear product $ш\colon \mathfrak{H}\times\mathfrak{H}\to\mathfrak{H}$ given by

$$1 \,ш\, w = w \,ш\, 1 = w,$$
$$uw \,ш\, u'w' = u(w \,ш\, u'w') + u'(uw \,ш\, w'),$$

where $w, w' \in \mathfrak{H}$ and $u, u' \in \{x, y\}$. This product makes $\mathfrak{H}$ a commutative $\mathbb{Q}$-algebra, which we denote by $\mathfrak{H}_ш$ (see [15]). The subspaces $\mathfrak{H}^1$ and $\mathfrak{H}^0$ become subalgebras of $\mathfrak{H}_ш$, which we denote by $\mathfrak{H}^1_ш$ and $\mathfrak{H}^0_ш$, respectively.

For a positive integer k, put $z_k = yx^{k-1}$. We define the $\mathbb{Q}$-linear map $Z\colon \mathfrak{H}^0\to\mathbb{R}$ by

$$Z(z_{k_1}\cdots z_{k_r}) = \zeta(k_1,\dots,k_r),$$

where $(k_1,\dots,k_r)$ is an admissible index. Note that Z is a ш-homomorphism in the sense that $Z(w_1 \,ш\, w_2) = Z(w_1)Z(w_2)$ for $w_1, w_2 \in \mathfrak{H}^0$.

We define the algebra homomorphism $\mathrm{reg}_ш : \mathfrak{H}_ш \to \mathfrak{H}^0_ш$ by the properties that it is the identity on $\mathfrak{H}^0$, maps x to 0, and maps y to 0; such $\mathrm{reg}_ш$ exists and is unique. We also define $Z^ш : \mathfrak{H}_ш\to\mathbb{R}$ by

$$Z^ш = Z\circ \mathrm{reg}_ш .$$

PROPOSITION 2.1. *For a nonnegative integer m and positive integers $k_1,\dots,k_r$, we have*

$$x^m yx^{k_1-1}\cdots yx^{k_r-1} \equiv (-1)^m \sum_{\substack{l_1,\dots,l_r\ge 0\\ l_1+\cdots+l_r=m}} yx^{k_1+l_1-1}\cdots yx^{k_r+l_r-1}\prod_{j=1}^{r}\binom{k_j+l_j-1}{l_j}$$

modulo $x \,ш\, \mathfrak{H}$.

Proof. Note that induction shows

$$x^m yw = \sum_{i=0}^{m}(-1)^{m-i}x^i \,ш\, y(x^{m-i} \,ш\, w)$$

for all $w \in \mathfrak{H}$. Indeed, the statement is obvious for $m = 0$, and if it is true for up to m, then

$$\begin{aligned} x^{m+1}yw &= x^{m+1} \,ш\, yw - \sum_{j=0}^{m} x^j y(x^{m+1-j} \,ш\, w) \\ &= x^{m+1} \,ш\, yw - \sum_{j=0}^{m}\sum_{i=0}^{j}(-1)^{j-i}x^i \,ш\, y(x^{j-i} \,ш\, x^{m+1-j} \,ш\, w) \end{aligned}$$

$$= x^{m+1} ш yw - \sum_{0\le i\le j\le m} (-1)^{j-i}\binom{m+1-i}{j-i} x^i ш y(x^{m+1-i} ш w)$$
$$= x^{m+1} ш yw + \sum_{i=0}^{m} (-1)^{m+1-i} x^i ш y(x^{m+1-i} ш w)$$
$$= \sum_{i=0}^{m+1} (-1)^{m+1-i} x^i ш y(x^{m+1-i} ш w).$$

Setting $w = x^{k_1-1}yx^{k_2-1}\cdots yx^{k_r-1}$, we have

$$\begin{aligned} x^m yx^{k_1-1}&\cdots yx^{k_r-1} \\ &= x^m yw \equiv (-1)^m y(x^m ш w) \\ &= (-1)^m \sum_{\substack{l_1,\dots,l_r\ge 0\\ l_1+\cdots+l_r=m}} yx^{k_1+l_1-1}\cdots yx^{k_r+l_r-1}\prod_{j=1}^{r}\binom{k_j+l_j-1}{l_j} \end{aligned}$$

modulo $x ш \mathfrak{H}$. ■

From the previous proposition and the observation that $x ш \mathfrak{H}$ lies in the kernel of $Z^{ш}$, we immediately deduce the following.

Proposition 2.2. *For a nonnegative integer m and positive integers $k_1,\dots,k_r$, we have*

$$\zeta^{ш}_m(k_1,\dots,k_r) = (-1)^m Z^{ш}(x^m yx^{k_1-1}\cdots yx^{k_r-1}).$$

Proposition 2.3. *Let $\boldsymbol{k}$ be an index with no adjacent ones. Then*

$$\zeta^*(\boldsymbol{k}) = \zeta^{ш}(\boldsymbol{k}), \qquad \zeta^*_{\widehat{\mathcal{S}}}(\boldsymbol{k}) = \zeta^{ш}_{\widehat{\mathcal{S}}}(\boldsymbol{k}).$$

Proof. By [8, Theorem 1], we see that

$$\zeta^*(\boldsymbol{l},1) = \zeta^{ш}(\boldsymbol{l},1)$$

for an index $\boldsymbol{l}$ whose last component is greater than 1. Then the result follows immediately from the definitions. ■

Let τ be the anti-automorphism on $\mathfrak{H}$ with $\tau(x) = y$ and $\tau(y) = x$. Then the duality formula of MZVs says $Z(w) = Z(\tau(w))$ for $w \in \mathfrak{H}^0$, which is generalized as follows.

Proposition 2.4. *For $w \in \mathfrak{H}$, we have*

$$Z^{ш}(w) = Z^{ш}(\tau(w)).$$

Proof. Since $\mathrm{reg}_{ш}$ and τ commute, we have

$$Z^{ш}(w) = Z(\mathrm{reg}_{ш}(w)) = Z(\tau(\mathrm{reg}_{ш}(w))) = Z(\mathrm{reg}_{ш}(\tau(w))) = Z^{ш}(\tau(w)),$$

as required. ■

2.2. Alternating sums of shuffle products. In this subsection, we compute several alternating sums of shuffle products to be used later in the proofs of the main theorems.

LEMMA 2.5. *For a nonnegative integer n, we have*

$$\sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} (yx)^{n-i} = \begin{cases}(-1)^{n/2}2^n x(y^2x^2)^{n/2} & \text{if } n \text{ is even},\\ (-1)^{(n-1)/2}2^n y(x^2y^2)^{(n-1)/2}x^2 & \text{if } n \text{ is odd}.\end{cases}$$

Proof. Put $a_n = \sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} (yx)^{n-i}$. If $n \geq 1$, we have

$$\begin{aligned} a_n &= xy\sum_{i=1}^{n}(-1)^i x(yx)^{i-1} \mathbin{ш} (yx)^{n-i} + xy\sum_{i=0}^{n-1}(-1)^i (yx)^i \mathbin{ш} x(yx)^{n-i-1} \\ &\quad + yx\sum_{i=0}^{n-1}(-1)^i (yx)^i \mathbin{ш} x(yx)^{n-i-1} + yx\sum_{i=0}^{n-1}(-1)^i x(yx)^i \mathbin{ш} (yx)^{n-i-1} \\ &= \big(-(1+(-1)^n)xy + (1-(-1)^n)yx\big)a_{n-1}. \end{aligned}$$

Since $a_0 = x$, we obtain the result by induction on n. ∎

LEMMA 2.6. *For a nonnegative integer n, we have*

$$\sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} (xy)^{n-i} = \begin{cases}(-1)^{n/2}2^n (x^2y^2)^{n/2}x & \text{if } n \text{ is even},\\ (-1)^{(n-1)/2}2^n x^2(y^2x^2)^{(n-1)/2}y & \text{if } n \text{ is odd}.\end{cases}$$

Proof. By looking at the reversal of both sides of the formula in Lemma 2.5, we find the result. ∎

LEMMA 2.7. *For a nonnegative integer n, we have*

$$\begin{aligned} &\sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} (yx)^{n-i}y \\ &= \begin{cases}(-1)^{n/2}2^n (x(y^2x^2)^{n/2}y + (yx^2y)^{n/2}yx) & \text{if } n \text{ is even},\\ (-1)^{(n-1)/2}2^n (-xy^2(x^2y^2)^{(n-1)/2}x + y(x^2y^2)^{(n-1)/2}x^2y) & \text{if } n \text{ is odd}.\end{cases} \end{aligned}$$

Proof. Let a_n and a'_n be the left-hand sides of the formulas in Lemmas 2.5 and 2.6, respectively. Then

$$\sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} (yx)^{n-i}y = (-1)^n x\tau(a_n) + ya'_n.$$

Thus the claim follows from those lemmas. ∎

LEMMA 2.8. *For a nonnegative integer n, we have*

$$\sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} x(yx)^{n-i} = \begin{cases}(-1)^{n/2}2^{n+1} x^2(y^2x^2)^{n/2} & \text{if } n \text{ is even},\\ 0 & \text{if } n \text{ is odd}.\end{cases}$$

Proof. Let a_n be the left-hand side of the formula in Lemma 2.5. Then

$$\sum_{i=0}^{n}(-1)^i x(yx)^i \mathbin{ш} x(yx)^{n-i} = (1+(-1)^n)xa_n.$$

Thus the claim follows from that lemma. ∎

2.3. Harmonic product and multiple zeta-star values. Let $\mathcal{I}$ be the $\mathbb{Q}$-vector space freely generated by all indices. We define the $\mathbb{Q}$-bilinear product $*$ on $\mathcal{I}$ inductively by setting

$$\boldsymbol{k} * \emptyset = \emptyset * \boldsymbol{k} = \boldsymbol{k},$$
$$(\boldsymbol{k}, k) * (\boldsymbol{l}, l) = (\boldsymbol{k} * (\boldsymbol{l}, l), k) + (\boldsymbol{k} * \boldsymbol{l}, k+l) + ((\boldsymbol{k}, k) * \boldsymbol{l}, l)$$

for all indices $\boldsymbol{k}$, $\boldsymbol{l}$ and all positive integers k, l. Note that $\zeta(\boldsymbol{k} * \boldsymbol{l}) = \zeta(\boldsymbol{k})\zeta(\boldsymbol{l})$ for any indices $\boldsymbol{k}$ and $\boldsymbol{l}$ whose last component is grater than 1.

For each admissible index $\boldsymbol{k} = (k_1, \dots, k_r)$, the *multiple zeta-star value* (*MZSV*) is defined by

$$\zeta^\star(\boldsymbol{k}) = \zeta^\star(k_1, \dots, k_r) = \sum_{1 \le n_1 \le \dots \le n_r} \frac{1}{n_1^{k_1} \cdots n_r^{k_r}} \in \mathbb{R},$$

where we set $\zeta^\star(\emptyset) = 1$. It is well known that

$$\sum_{i=0}^{r}(-1)^i \zeta(k_1, \dots, k_i)\zeta^\star(k_r, \dots, k_{i+1}) = \delta_{r,0}$$

for every index $\boldsymbol{k} = (k_1, \dots, k_r)$ satisfying $k_1, \dots, k_r \ge 2$; this will be referred to as the *antipode formula* in connection with the antipode property in a Hopf algebra.

2.4. Computation of generating series. In this subsection, we compute several generating series to be used later in the proof of our main theorems. It turns out that all generating series we will need can be expressed in terms of the four generating series $F_+, F_-, G_+, G_- \in \mathbb{R}[[u]]$ defined by

$$F_\pm = \sum_{n \ge 0}(\pm 2)^{-n}\zeta(2n+1)u^{2n+1}, \qquad G_\pm = \sum_{n \ge 0}(\pm 2)^{-n}\zeta(\{2\}^n)u^{2n}.$$

Observe that

$$F_+ + F_- = 2\sum_{\substack{n \ge 0 \\ n\,\text{even}}} 2^{-n}\zeta(2n+1)u^{2n+1} = 2\sum_{n \ge 0} 4^{-n}\zeta(4n+1)u^{4n+1},$$

$$F_+ - F_- = 2\sum_{\substack{n \ge 0 \\ n\,\text{odd}}} 2^{-n}\zeta(2n+1)u^{2n+1} = \sum_{n \ge 0} 4^{-n}\zeta(4n+3)u^{4n+3},$$

$$G_+ + G_- = 2\sum_{\substack{n \ge 0 \\ n\,\text{even}}} 2^{-n}\zeta(\{2\}^n)u^{2n} = 2\sum_{n \ge 0} 4^{-n}\zeta(\{2\}^{2n})u^{4n},$$

$$G_+ - G_- = 2\sum_{\substack{n\geq 0\\ n\,\mathrm{odd}}} 2^{-n}\zeta(\{2\}^n)u^{2n} = \sum_{n\geq 0} 4^{-n}\zeta(\{2\}^{2n+1})u^{4n+2},$$

and that

$$\sum_{n\geq 0}(\pm 2)^{-n}\zeta^\star(\{2\}^n)u^{2n} = G_\mp^{-1}$$

by the antipode formula.

Lemma 2.9. *We have*

$$\begin{aligned} G_+G_- &= \sum_{n\geq 0}(-1)^n\zeta(\{1,3\}^n)u^{4n} = \sum_{n\geq 0}(-4)^{-n}\zeta(\{4\}^n)u^{4n} \\ &= \Bigl(\sum_{n\geq 0}4^{-n}\zeta^\star(\{4\}^n)u^{4n}\Bigr)^{-1} \end{aligned}$$

and

$$G_\pm^2 = \sum_{n\geq 0}\frac{(\pm 1)^n 2^{n+1}\pi^{2n}}{(2n+2)!}u^{2n}, \qquad \frac{G_+^2+G_-^2}{2} = \sum_{n\geq 0}\zeta(\{4\}^n)u^{4n}.$$

Proof. Recall that

$$\zeta(\{2\}^n) = \frac{\pi^{2n}}{(2n+1)!}, \qquad \zeta(\{1,3\}^n) = \frac{2\pi^{4n}}{(4n+2)!}, \qquad \zeta(\{4\}^n) = \frac{2^{2n+1}\pi^{4n}}{(4n+2)!}$$

for every nonnegative integer n (see Borwein, Bradley, Broadhurst, and Lisoněk [5, Example 2.2] for the last two identities). It follows that

$$\begin{aligned} G_+G_- &= \Bigl(\sum_{n_1\geq 0}\frac{1}{(2n_1+1)!}\Bigl(\frac{\pi^2u^2}{2}\Bigr)^{n_1}\Bigr)\Bigl(\sum_{n_2\geq 0}\frac{(-1)^{n_2}}{(2n_2+1)!}\Bigl(\frac{\pi^2u^2}{2}\Bigr)^{n_2}\Bigr) \\ &= \sum_{n\geq 0}\Bigl(\sum_{\substack{n_1+n_2=n\\ n_1,n_2\geq 0}}\frac{(-1)^{n_2}}{(2n_1+1)!(2n_2+1)!}\Bigr)\Bigl(\frac{\pi^2u^2}{2}\Bigr)^n \\ &= \sum_{n\geq 0}\frac{\mathrm{Im}((1+i)^{2n+2})}{(2n+2)!}\Bigl(\frac{\pi^2u^2}{2}\Bigr)^n \qquad \text{(binomial theorem)} \\ &= \sum_{\substack{n\geq 0\\ n\,\mathrm{even}}}\frac{(-1)^{n/2}2^{n+1}}{(2n+2)!}\Bigl(\frac{\pi^2u^2}{2}\Bigr)^n = \sum_{n\geq 0}\frac{2(-1)^n\pi^{4n}}{(4n+2)!}u^{4n}, \end{aligned}$$

which together with the antipode formula implies that

$$\begin{aligned} G_+G_- &= \sum_{n\geq 0}(-1)^n\zeta(\{1,3\}^n)u^{4n} = \sum_{n\geq 0}(-4)^{-n}\zeta(\{4\}^n)u^{4n} \\ &= \Bigl(\sum_{n\geq 0}4^{-n}\zeta^\star(\{4\}^n)u^{4n}\Bigr)^{-1}. \end{aligned}$$

We also have

$$\begin{aligned}
G_{\pm}^2 &= \Biggl(\sum_{n_1\geq 0}\frac{1}{(2n_1+1)!}\Bigl(\pm\frac{\pi^2u^2}{2}\Bigr)^{n_1}\Biggr)\Biggl(\sum_{n_2\geq 0}\frac{1}{(2n_2+1)!}\Bigl(\pm\frac{\pi^2u^2}{2}\Bigr)^{n_2}\Biggr)\\
&= \sum_{n\geq 0}\Biggl(\sum_{\substack{n_1+n_2=n\\ n_1,n_2\geq 0}}\frac{1}{(2n_1+1)!(2n_2+1)!}\Biggr)\Bigl(\pm\frac{\pi^2u^2}{2}\Bigr)^{n}\\
&= \sum_{n\geq 0}\frac{2^{2n+1}}{(2n+2)!}\Bigl(\pm\frac{\pi^2u^2}{2}\Bigr)^{n} \qquad \text{(binomial theorem)}\\
&= \sum_{n\geq 0}\frac{(\pm 1)^n 2^{n+1}\pi^{2n}}{(2n+2)!}u^{2n},
\end{aligned}$$

which implies that

$$\frac{G_+^2+G_-^2}{2} = \sum_{\substack{n\geq 0\\ n\,\text{even}}}\frac{2^{n+1}\pi^{2n}}{(2n+2)!}u^{2n} = \sum_{n\geq 0}\frac{2^{2n+1}\pi^{4n}}{(4n+2)!}u^{4n} = \sum_{n\geq 0}\zeta(\{4\}^n)u^{4n}. \blacksquare$$

Lemma 2.10. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta(\{3,1\}^n,3)u^{4n+3} = (F_+-F_-)G_+G_-.$$

Proof. Bowman and Bradley [6, Theorem 1] showed that

$$\zeta(\{3,1\}^n,3) = 4^{-n}\sum_{i=0}^{n}(-1)^i\zeta(4i+3)\zeta(\{4\}^{n-i})$$

for every nonnegative integer n. It follows that

$$\begin{aligned}
&\sum_{n\geq 0}(-1)^n\zeta(\{3,1\}^n,3)u^{4n+3}\\
&\qquad= \sum_{n\geq 0}(-4)^{-n}\sum_{i=0}^{n}(-1)^i\zeta(4i+3)\zeta(\{4\}^{n-i})u^{4n+3}\\
&\qquad= \Bigl(\sum_{n_1\geq 0}4^{-n_1}\zeta(4n_1+3)u^{4n_1+3}\Bigr)\Bigl(\sum_{n_2\geq 0}(-4)^{-n_2}\zeta(\{4\}^{n_2})u^{4n_2}\Bigr)\\
&\qquad= (F_+-F_-)G_+G_-
\end{aligned}$$

by Lemma 2.9. ■

Lemma 2.11. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta(\{1,3\}^n,1)u^{4n+1} = (F_++F_-)G_+G_-.$$

Proof. Bachmann and Charlton [1, Proposition 4.2] showed that

$$\zeta(\{1,3\}^n,1) = 2^{-2n+1}\sum_{i=0}^{n}(-1)^i\zeta(4i+1)\zeta(\{4\}^{n-i})$$

for every nonnegative integer n (note that the summand is equal to 0 if $i=0$). It follows that

$$\begin{aligned}
&\sum_{n\geq 0}(-1)^n\zeta(\{1,3\}^n,1)u^{4n+1}\\
&\qquad = 2\sum_{n\geq 0}(-4)^{-n}\sum_{i=0}^{n}(-1)^i\zeta(4i+1)\zeta(\{4\}^{n-i})u^{4n+1}\\
&\qquad = \Big(2\sum_{n_1\geq 0}4^{-n_1}\zeta(4n_1+1)u^{4n_1+1}\Big)\Big(\sum_{n_2\geq 0}(-4)^{-n_2}\zeta(\{4\}^{n_2})u^{4n_2}\Big)\\
&\qquad = (F_+ + F_-)G_+G_-
\end{aligned}$$

by Lemma 2.9. ■

LEMMA 2.12. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta(\{3,1\}^n)u^{4n} = \frac{G_+^2+G_-^2}{2G_+G_-} - (F_+^2 - F_-^2)G_+G_-.$$

Proof. Bachmann and Charlton [1, Proposition 4.2] showed that

$$\begin{aligned}
\zeta(\{3,1\}^n) &= (-1)^n\sum_{i=0}^{n}4^{-i}\zeta^\star(\{4\}^i)\zeta(\{4\}^{n-i})\\
&\qquad + 2^{-2n+3}\sum_{\substack{1\leq i\leq n-1\\ 0\leq j\leq n-i-1}}(-1)^{i+j}\zeta(4i+1)\zeta(4j+3)\zeta(\{4\}^{n-i-j-1})
\end{aligned}$$

for every nonnegative integer n. It follows that

$$\begin{aligned}
&\sum_{n\geq 0}(-1)^n\zeta(\{3,1\}^n)u^{4n}\\
&= \sum_{n\geq 0}\sum_{i=0}^{n}4^{-i}\zeta^\star(\{4\}^i)\zeta(\{4\}^{n-i})u^{4n}\\
&\quad - 2\sum_{n\geq 0}(-4)^{-(n-1)}\sum_{\substack{1\leq i\leq n-1\\ 0\leq j\leq n-i-1}}(-1)^{i+j}\zeta(4i+1)\zeta(4j+3)\zeta(\{4\}^{n-i-j-1})u^{4n}\\
&= \Big(\sum_{n_1\geq 0}4^{-n_1}\zeta^\star(\{4\}^{n_1})u^{4n_1}\Big)\Big(\sum_{n_2\geq 0}\zeta(\{4\}^{n_2})u^{4n_2}\Big)\\
&\quad - \Big(2\sum_{n_1\geq 0}4^{-n_1}\zeta(4n_1+1)u^{4n_1+1}\Big)\Big(\sum_{n_2\geq 0}4^{-n_2}\zeta(4n_2+3)u^{4n_2+3}\Big)\\
&\qquad\qquad \times\Big(\sum_{n_3\geq 0}(-4)^{-n_3}\zeta(\{4\}^{n_3})u^{4n_3}\Big)
\end{aligned}$$

$$= G_+^{-1}G_-^{-1}\frac{G_+^2+G_-^2}{2} - (F_+ + F_-)(F_+ - F_-)G_+G_- \qquad \text{(Lemma 2.9)}$$
$$= \frac{G_+^2+G_-^2}{2G_+G_-} - (F_+^2 - F_-^2)G_+G_-. \ \blacksquare$$

LEMMA 2.13. *We have*

$$\sum_{n\geq 0} 4^{-n}(4n+1)\zeta(4n+2)u^{4n+2} = \frac{G_-^{-2} - G_+^{-2}}{2}.$$

Proof. Since

$$\Big(\sum_{n\geq 0}\zeta^\star(\{2\}^n)v^{2n}\Big)^2 = \Big(\frac{\pi v}{\sin(\pi v)}\Big)^2 = -\pi v^2 \frac{d}{dv}\cot(\pi v)$$
$$= 2v^2\frac{d}{dv}\sum_{n\geq 0}\zeta(2n)v^{2n-1} = 2\sum_{n\geq 0}(2n-1)\zeta(2n)v^{2n}$$

(here we set $\zeta(0) = -1/2$), setting $v^2 = \mp u^2/2$ we have

$$G_\pm^{-2} = 2\sum_{n\geq 0}(\mp 2)^{-n}(2n-1)\zeta(2n)u^{2n}.$$

Then we get

$$G_-^{-2} - G_+^{-2} = 4\sum_{\substack{n\geq 0\\ n\,\mathrm{odd}}} 2^{-n}(2n-1)\zeta(2n)u^{2n} = 2\sum_{n\geq 0}4^{-n}(4n+1)\zeta(4n+2)u^{4n+2},$$

as required. $\blacksquare$

LEMMA 2.14. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta(\{3,1\}^n,2)u^{4n+2} = \frac{G_+^2 - G_-^2}{2G_+G_-} - (F_+ - F_-)^2G_+G_-.$$

Proof. Bowman and Bradley [6, Theorem 2] showed that

$$\zeta(\{3,1\}^n,2)$$
$$= 4^{-n}\sum_{i=0}^{n}(-1)^i\zeta(\{4\}^{n-i})\Big((4i+1)\zeta(4i+2) - 4\sum_{j=1}^{i}\zeta(4j-1)\zeta(4i-4j+3)\Big)$$

for every nonnegative integer n. It follows that

$$\sum_{n\geq 0}(-1)^n\zeta(\{3,1\}^n,2)u^{4n+2}$$
$$= \sum_{n\geq 0}(-4)^{-n}\sum_{i=0}^{n}(-1)^i\zeta(\{4\}^{n-i})(4i+1)\zeta(4i+2)u^{4n+2}$$
$$- 4\sum_{n\geq 0}(-4)^{-n}\sum_{i=0}^{n}(-1)^i\zeta(\{4\}^{n-i})\sum_{j=1}^{i}\zeta(4j-1)\zeta(4i-4j+3)u^{4n+2}$$

$$= \Big(\sum_{n_1\geq 0}(-4)^{-n_1}\zeta(\{4\}^{n_1})u^{4n_1}\Big)\Big(\sum_{n_2\geq 0}4^{-n_2}(4n_2+1)\zeta(4n_2+2)u^{4n_2+2}\Big)$$

$$- \Big(\sum_{n_1\geq 0}(-4)^{-n_1}\zeta(\{4\}^{n_1})u^{4n_1}\Big)\Big(\sum_{n_2\geq 0}4^{-n_2}\zeta(4n_2+3)u^{4n_2+3}\Big) \times \Big(\sum_{n_3\geq 0}4^{-n_3}\zeta(4n_3+3)u^{4n_3+3}\Big)$$

$$= G_+G_-\cdot\frac{G_-^{-2}-G_+^{-2}}{2} - G_+G_-(F_+-F_-)^2 \quad \text{(Lemmas 2.9 and 2.13)}$$

$$= \frac{G_+^2-G_-^2}{2G_+G_-} - (F_+-F_-)^2G_+G_-. \ \blacksquare$$

LEMMA 2.15. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta_1(\{1,3\}^n)u^{4n+1} = -(F_+ + F_-)G_+G_-.$$

Proof. Since Propositions 2.2 and 2.4 show that

$$\zeta_1(\{1,3\}^n) = -Z^{ш}(x(y^2x^2)^n) = -Z^{ш}((y^2x^2)^n y) = -\zeta(\{1,3\}^n,1)$$

for every nonnegative integer n, the lemma follows from Lemma 2.11. ∎

Let $\widetilde{ш}$ denote the shuffle of indices, e.g., $(a,b)\,\widetilde{ш}\,(c) = (a,b,c)+(a,c,b)+(c,a,b)$.

LEMMA 2.16. *If a and b are positive integers, then*

$$\sum_{i=0}^{n}(-1)^i(ai+b)*(\{a\}^{n-i}) = (b)\,\widetilde{ш}\,(\{a\}^n)$$

for every nonnegative integer n.

Proof. We have

$$\sum_{i=0}^{n}(-1)^i(ai+b)*(\{a\}^{n-i})$$

$$= \sum_{i=0}^{n-1}(-1)^i\big((ai+b)\,\widetilde{ш}\,(\{a\}^{n-i}) + (a(i+1)+b)\,\widetilde{ш}\,(\{a\}^{n-i-1})\big)$$

$$+ (-1)^n(an+b)$$

$$= (b)\,\widetilde{ш}\,(\{a\}^n),$$

as required. ∎

LEMMA 2.17. *We have*

$$\zeta_1(\{2\}^n) = -2\sum_{i=0}^{n}(-1)^i\zeta(2i+1)\zeta(\{2\}^{n-i})$$

for every nonnegative integer n.

Proof. We have

$$\begin{aligned}\zeta_1(\{2\}^n) &= \binom{2+1-1}{1}\sum_{i=1}^{n}\zeta(\{2\}^{i-1},3,\{2\}^{n-i})\\ &= 2\zeta((1)*(\{2\}^n)-(1)\,\widetilde{ш}\,(\{2\}^n)) = -2\zeta((1)\,\widetilde{ш}\,(\{2\}^n))\\ &= -2\sum_{i=0}^{n}(-1)^i\zeta(2i+1)\zeta(\{2\}^{n-i})\end{aligned}$$

by Lemma 2.16 with $a=2$ and $b=1$. ∎

LEMMA 2.18. *We have*

$$\sum_{n\geq 0}(\pm 2)^{-n}\zeta_1(\{2\}^n)u^{2n+1} = -2F_{\mp}G_{\pm}.$$

Proof. Lemma 2.17 implies that

$$\begin{aligned}&\sum_{n\geq 0}(\pm 2)^{-n}\zeta_1(\{2\}^n)u^{2n+1}\\ &\quad= -2\sum_{n\geq 0}(\pm 2)^{-n}\sum_{i=0}^{n}(-1)^i\zeta(2i+1)\zeta(\{2\}^{n-i})u^{2n+1}\\ &\quad= -2\Big(\sum_{n_1\geq 0}(\mp 2)^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_2\geq 0}(\pm 2)^{-n_2}\zeta(\{2\}^{n_2})u^{2n_2}\Big)\\ &\quad= -2F_{\mp}G_{\pm}. \ \blacksquare\end{aligned}$$

LEMMA 2.19. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta_1(\{1,3\}^n,1)u^{4n+2} = \frac{G_+^2-G_-^2}{2G_+G_-}-(F_++F_-)^2G_+G_-.$$

Proof. Propositions 2.2 and 2.4 and Lemma 2.7 show that

$$\begin{aligned}&\sum_{i=0}^{n}(-1)^i\zeta_1(\{2\}^i)\zeta_1(\{2\}^{n-i})\\ &\quad= \sum_{i=0}^{n}(-1)^iZ^{ш}(x(yx)^i)Z^{ш}(x(yx)^{n-i})\\ &\quad= \sum_{i=0}^{n}(-1)^iZ^{ш}(x(yx)^i)Z^{ш}((yx)^{n-i}y)\\ &\quad= \begin{cases}(-1)^{n/2}2^n(Z^{ш}(x(y^2x^2)^{n/2}y)+Z^{ш}((yx^2y)^{n/2}yx)) & \text{if } n \text{ is even},\\ (-1)^{(n-1)/2}2^n\big(-Z^{ш}(xy^2(x^2y^2)^{(n-1)/2}x)+Z^{ш}(y(x^2y^2)^{(n-1)/2}x^2y)\big) & \\ & \text{if } n \text{ is odd}\end{cases}\\ &\quad= \begin{cases}(-1)^{n/2}2^n\big(-\zeta_1(\{1,3\}^{n/2},1)+\zeta(\{3,1\}^{n/2},2)\big) & \text{if } n \text{ is even},\\ 0 & \text{if } n \text{ is odd}.\end{cases}\end{aligned}$$

It follows that

$$\begin{aligned}
&\sum_{n\ge 0}(-1)^n\bigl(-\zeta_1(\{1,3\}^n,1)+\zeta(\{3,1\}^n,2)\bigr)u^{4n+2}\\
&\quad=\sum_{\substack{n\ge 0\\ n\,\text{even}}}(-1)^{n/2}\bigl(-\zeta_1(\{1,3\}^{n/2},1)+\zeta(\{3,1\}^{n/2},2)\bigr)u^{2n+2}\\
&\quad=\sum_{n\ge 0}2^{-n}\sum_{i=0}^{n}(-1)^i\zeta_1(\{2\}^i)\zeta_1(\{2\}^{n-i})u^{2n+2}\\
&\quad=\Bigl(\sum_{n_1\ge 0}(-2)^{-n_1}\zeta_1(\{2\}^{n_1})u^{2n_1+1}\Bigr)\Bigl(\sum_{n_2\ge 0}2^{-n_2}\zeta_1(\{2\}^{n_2})u^{2n_2+1}\Bigr)\\
&\quad=(-2F_+G_-)(-2F_-G_+)\qquad\text{(Lemma 2.18)}\\
&\quad=4F_+F_-G_+G_-.
\end{aligned}$$

Using Lemma 2.14, we infer that

$$\begin{aligned}
\sum_{n\ge 0}(-1)^n\zeta_1(\{1,3\}^n,1)u^{4n+2}&=\sum_{n\ge 0}(-1)^n\zeta(\{3,1\}^n,2)u^{4n+2}-4F_+F_-G_+G_-\\
&=\frac{G_+^2-G_-^2}{2G_+G_-}-(F_+-F_-)^2G_+G_--4F_+F_-G_+G_-\\
&=\frac{G_+^2-G_-^2}{2G_+G_-}-(F_++F_-)^2G_+G_-. \qquad ■
\end{aligned}$$

Lemma 2.20. *We have*

$$\sum_{n\ge 0}(-1)^n\zeta_2(\{1,3\}^n)u^{4n+2}=2F_+F_-G_+G_-.$$

Proof. We have

$$\begin{aligned}
&\sum_{n\ge 0}(-1)^n\zeta_2(\{1,3\}^n)u^{4n+2}\\
&\quad=\sum_{n\ge 0}(-1)^nZ^{ш}(x^2(y^2x^2)^n)u^{4n+2}\qquad\text{(Proposition 2.2)}\\
&\quad=\sum_{\substack{n\ge 0\\ n\,\text{even}}}(-1)^{n/2}Z^{ш}(x^2(y^2x^2)^{n/2})u^{2n+2}\\
&\quad=\sum_{n\ge 0}2^{-n-1}\sum_{i=0}^{n}(-1)^iZ^{ш}(x(yx)^i)Z^{ш}(x(yx)^{n-i})u^{2n+2}\qquad\text{(Lemma 2.8)}\\
&\quad=\sum_{n\ge 0}2^{-n-1}\sum_{i=0}^{n}(-1)^i\zeta_1(\{2\}^i)\zeta_1(\{2\}^{n-i})u^{2n+2}\qquad\text{(Proposition 2.2)}
\end{aligned}$$

$$= 2^{-1}\Big(\sum_{n_1\geq 0}(-2)^{-n_1}\zeta_1(\{2\}^{n_1})u^{2n_1+1}\Big)\Big(\sum_{n_2\geq 0}2^{-n_2}\zeta_1(\{2\}^{n_2})u^{2n_2+1}\Big)$$
$$= 2^{-1}(-2F_+G_-)(-2F_-G_+) \quad \text{(Lemma 2.18)}$$
$$= 2F_+F_-G_+G_-. \blacksquare$$

LEMMA 2.21. *We have*

$$\sum_{n\geq 0}(\pm 2)^{-n}Z^{ш}((xy)^n)u^{2n} = G_{\pm}^{-1} \pm 2F_{\mp}^2 G_{\pm}.$$

Proof. We have

$$\begin{aligned}\delta_{n,0} &= 1 ш (xy)^n - y ш (xy)^{n-1}x + yx ш (xy)^{n-1} - \cdots \\ &\quad - (yx)^{n-1}y ш x + (yx)^n ш 1 \\ &= \sum_{i=0}^{n}(yx)^i ш (xy)^{n-i} - \sum_{i=1}^{n}(yx)^{i-1}y ш (xy)^{n-i}x\end{aligned}$$

for every nonnegative integer n. It follows that

$$\begin{aligned}1 &= \sum_{n\geq 0}(\pm 2)^{-n}\delta_{n,0}u^{2n} \\ &= \sum_{n\geq 0}(\pm 2)^{-n}\Big(\sum_{i=0}^{n}Z^{ш}((yx)^i)Z^{ш}((xy)^{n-i}) \\ &\qquad\qquad - \sum_{i=1}^{n}Z^{ш}((yx)^{i-1}y)Z^{ш}((xy)^{n-i}x)\Big)u^{2n} \\ &= \sum_{n\geq 0}(\pm 2)^{-n}\Big(\sum_{i=0}^{n}\zeta(\{2\}^i)Z^{ш}((xy)^{n-i}) - \sum_{i=1}^{n}\zeta_1(\{2\}^{i-1})\zeta_1(\{2\}^{n-i})\Big)u^{2n} \\ &\qquad\qquad \text{(Propositions 2.2 and 2.4)} \\ &= \Big(\sum_{n_1\geq 0}(\pm 2)^{-n_1}\zeta(\{2\}^{n_1})u^{2n_1}\Big)\Big(\sum_{n_2\geq 0}(\pm 2)^{-n_2}Z^{ш}((xy)^{n_2})u^{2n_2}\Big) \\ &\quad \mp 2^{-1}\Big(\sum_{n_1\geq 0}(\pm 2)^{-n_1}\zeta_1(\{2\}^{n_1})u^{2n_1+1}\Big)\Big(\sum_{n_2\geq 0}(\pm 2)^{-n_2}\zeta_1(\{2\}^{n_2})u^{2n_2+1}\Big) \\ &= G_{\pm}\sum_{n\geq 0}(\pm 2)^{-n}Z^{ш}((xy)^n)u^{2n} \mp 2^{-1}(-2F_{\mp}G_{\pm})^2 \quad \text{(Lemma 2.18)} \\ &= G_{\pm}\sum_{n\geq 0}(\pm 2)^{-n}Z^{ш}((xy)^n)u^{2n} \mp 2F_{\mp}^2G_{\pm}^2. \blacksquare\end{aligned}$$

LEMMA 2.22. *We have*

$$\sum_{n\geq 0}(-1)^n\zeta_2(\{1,3\}^n,1)u^{4n+3} = \frac{F_+G_-^2 - F_-G_+^2}{G_+G_-} + 2F_+F_-(F_+ + F_-)G_+G_-.$$

Proof. We have

$$\begin{aligned}
&\sum_{n\geq 0}(-1)^n\zeta_2(\{1,3\}^n,1)u^{4n+3}\\
&=\sum_{n\geq 0}(-1)^n Z^{ш}(x^2(y^2x^2)^n y)u^{4n+3} \quad \text{(Proposition 2.2)}\\
&=\sum_{n\geq 0}2^{-2n-1}\sum_{i=0}^{2n+1}(-1)^i Z^{ш}(x(yx)^i)Z^{ш}((xy)^{2n-i+1})u^{4n+3} \quad \text{(Lemma 2.6)}\\
&=-\sum_{n\geq 0}2^{-2n-1}\sum_{i=0}^{2n+1}(-1)^i\zeta_1(\{2\}^i)Z^{ш}((xy)^{2n-i+1})u^{4n+3} \quad \text{(Proposition 2.2)}\\
&=-\sum_{\substack{n_1,n_2\geq 0\\ n_1+n_2 \text{ odd}}}2^{-n_1-n_2}(-1)^{-n_1}\zeta_1(\{2\}^{n_1})Z^{ш}((xy)^{n_2})u^{2(n_1+n_2)+1}\\
&=-2^{-1}\sum_{n_1,n_2\geq 0}(1-(-1)^{n_1+n_2})2^{-n_1-n_2}(-1)^{-n_1}\zeta_1(\{2\}^{n_1})\\
&\qquad\qquad \times Z^{ш}((xy)^{n_2})u^{2(n_1+n_2)+1}\\
&=-2^{-1}\Bigg(\Big(\sum_{n_1\geq 0}(-2)^{-n_1}\zeta_1(\{2\}^{n_1})u^{2n_1+1}\Big)\Big(\sum_{n_2\geq 0}2^{-n_2}Z^{ш}((xy)^{n_2})u^{2n_2}\Big)\\
&\qquad -\Big(\sum_{n_1\geq 0}2^{-n_1}\zeta_1(\{2\}^{n_1})u^{2n_1+1}\Big)\Big(\sum_{n_2\geq 0}(-2)^{-n_2}Z^{ш}((xy)^{n_2})u^{2n_2}\Big)\Bigg)\\
&=-2^{-1}(-2F_+G_-(G_+^{-1}+2F_-^2G_+)+2F_-G_+(G_-^{-1}-2F_+^2G_-))\\
&\qquad \text{(Lemmas 2.18 and 2.21)}\\
&=\frac{F_+G_-^2-F_-G_+^2}{G_+G_-}+2F_+F_-(F_++F_-)G_+G_-. \qquad \blacksquare
\end{aligned}$$

2.5. Proofs of Theorems 1.3 and 1.5

Proof of Theorem 1.3. Since $\zeta_{\mathcal{S}_3}(\{3,1\}^n)$ equals

$$\sum_{i=0}^{n}\zeta(\{3,1\}^i)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i})t^m-\sum_{i=1}^{n}\zeta(\{3,1\}^{i-1},3)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i},1)t^m$$

for every nonnegative integer n, we have

$$\begin{aligned}
&\sum_{n\geq 0}(-1)^n\zeta_{\mathcal{S}_3}(\{3,1\}^n)u^{4n}\\
&\qquad =\sum_{n\geq 0}(-1)^n\sum_{i=0}^{n}\zeta(\{3,1\}^i)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i})t^m u^{4n}\\
&\qquad\quad -\sum_{n\geq 0}(-1)^n\sum_{i=1}^{n}\zeta(\{3,1\}^{i-1},3)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i},1)t^m u^{4n}
\end{aligned}$$

$$= \Big(\sum_{n_1\geq 0}(-1)^{n_1}\zeta(\{3,1\}^{n_1})u^{4n_1}\Big)\Big(\sum_{m=0}^{2}\sum_{n_2\geq 0}(-1)^{n_2}\zeta_m(\{1,3\}^{n_2})u^{4n_2}t^m\Big)$$

$$+\Big(\sum_{n_1\geq 0}(-1)^{n_1}\zeta(\{3,1\}^{n_1},3)u^{4n_1+3}\Big)$$

$$\times\Big(\sum_{m=0}^{2}\sum_{n_2\geq 0}(-1)^{n_2}\zeta_m(\{1,3\}^{n_2},1)u^{4n_2+1}t^m\Big)$$

$$= \left(\frac{G_+^2+G_-^2}{2G_+G_-}-(F_+^2-F_-^2)G_+G_-\right)$$

$$\times\left(G_+G_- -(F_++F_-)G_+G_-\frac{t}{u}+2F_+F_-G_+G_-\frac{t^2}{u^2}\right)$$

$$+(F_+-F_-)G_+G_-\left((F_++F_-)G_+G_-+\left(\frac{G_+^2-G_-^2}{2G_+G_-}-(F_++F_-)^2G_+G_-\right)\frac{t}{u}\right.$$

$$\left.+\left(\frac{F_+G_-^2-F_-G_+^2}{G_+G_-}+2F_+F_-(F_++F_-)G_+G_-\right)\frac{t^2}{u^2}\right)$$

$$= \frac{G_+^2+G_-^2}{2}-(F_+G_-^2+F_-G_+^2)\frac{t}{u}+(F_+^2G_-^2+F_-^2G_+^2)\frac{t^2}{u^2}$$

by Lemmas 2.9–2.12, 2.15, 2.19, 2.20, and 2.22.

Now since Lemma 2.9 implies that

$$\frac{G_+^2+G_-^2}{2}=\sum_{n\geq 0}\frac{2^{2n+1}\pi^{4n}}{(4n+2)!}u^{4n},$$

that

$$-(F_+G_-^2+F_-G_+^2)\frac{t}{u}$$

$$= -\Big(\sum_{n_1\geq 0}2^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_0\geq 0}\frac{(-1)^{n_0}2^{n_0+1}\pi^{2n_0}}{(2n_0+2)!}u^{2n_0}\Big)\frac{t}{u}$$

$$-\Big(\sum_{n_1\geq 0}(-2)^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_0\geq 0}\frac{2^{n_0+1}\pi^{2n_0}}{(2n_0+2)!}u^{2n_0}\Big)\frac{t}{u}$$

$$= -\sum_{n_0,n_1\geq 0}\frac{((-1)^{n_0}+(-1)^{n_1})2^{n_0-n_1+1}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)u^{2n_0+2n_1}t$$

$$= -\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1\ \text{even}}}\frac{(-1)^{n_0}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)u^{2n_0+2n_1}t,$$

and that

$$
\begin{aligned}
&(F_+^2G_-^2+F_-^2G_+^2)\frac{t^2}{u^2}\\
&=\Big(\sum_{n_1\ge0}2^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_2\ge0}2^{-n_2}\zeta(2n_2+1)u^{2n_2+1}\Big)\\
&\quad\times\Bigg(\sum_{n_0\ge0}\frac{(-1)^{n_0}2^{n_0+1}\pi^{2n_0}}{(2n_0+2)!}u^{2n_0}\Bigg)\frac{t^2}{u^2}\\
&\quad+\Big(\sum_{n_1\ge0}(-2)^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_2\ge0}(-2)^{-n_2}\zeta(2n_2+1)u^{2n_2+1}\Big)\\
&\qquad\qquad\qquad\qquad\qquad\times\Bigg(\sum_{n_0\ge0}\frac{2^{n_0+1}\pi^{2n_0}}{(2n_0+2)!}u^{2n_0}\Bigg)\frac{t^2}{u^2}\\
&=\sum_{n_0,n_1,n_2\ge0}\frac{((-1)^{n_0}+(-1)^{n_1+n_2})2^{n_0-n_1-n_2+1}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\zeta(2n_2+1)\\
&\qquad\qquad\qquad\qquad\qquad\times u^{2(n_0+n_1+n_2)}t^2\\
&=\sum_{\substack{n_0,n_1,n_2\ge0\\ n_0+n_1+n_2\text{ even}}}\frac{(-1)^{n_0}2^{n_0-n_1-n_2+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\zeta(2n_2+1)u^{2(n_0+n_1+n_2)}t^2,
\end{aligned}
$$

we have

$$
\begin{aligned}
&(-1)^n\zeta_{\mathcal{S}_3}(\{3,1\}^n)\\
&\quad=\frac{2^{2n+1}}{(4n+2)!}\pi^{4n}-\sum_{\substack{n_0,n_1\ge0\\ n_0+n_1=2n}}\frac{(-1)^{n_0}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)t\\
&\qquad+\sum_{\substack{n_0,n_1,n_2\ge0\\ n_0+n_1+n_2=2n}}\frac{(-1)^{n_0}2^{n_0-n_1-n_2+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\zeta(2n_2+1)t^2,
\end{aligned}
$$

from which the theorem follows. ■

Proof of Theorem 1.5. Since

$$
\begin{aligned}
\zeta_{\mathcal{S}_3}(\{1,3\}^n,1)=&-\sum_{i=0}^{n}\zeta(\{1,3\}^i)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i},1)t^m\\
&+\sum_{i=0}^{n}\zeta(\{1,3\}^i,1)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i})t^m
\end{aligned}
$$

for every nonnegative integer n, we have

$$
\begin{aligned}
&\sum_{n\geq 0}(-1)^n\zeta_{\mathcal{S}_3}(\{1,3\}^n,1)u^{4n+1}\\
&=-\sum_{n\geq 0}(-1)^n\sum_{i=0}^{n}\zeta(\{1,3\}^i)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i},1)t^m u^{4n+1}\\
&\quad+\sum_{n\geq 0}(-1)^n\sum_{i=0}^{n}\zeta(\{1,3\}^i,1)\sum_{m=0}^{2}\zeta_m(\{1,3\}^{n-i})t^m u^{4n+1}\\
&=-\Big(\sum_{n_1\geq 0}(-1)^{n_1}\zeta(\{1,3\}^{n_1})u^{4n_1}\Big)\Big(\sum_{m=0}^{2}\sum_{n_2\geq 0}(-1)^{n_2}\zeta_m(\{1,3\}^{n_2},1)u^{4n_2+1}t^m\Big)\\
&\quad+\Big(\sum_{n_1\geq 0}(-1)^{n_1}\zeta(\{1,3\}^{n_1},1)u^{4n_1+1}\Big)\Big(\sum_{m=0}^{2}\sum_{n_2\geq 0}(-1)^{n_2}\zeta_m(\{1,3\}^{n_2})u^{4n_2}t^m\Big)\\
&=-G_+G_-\Bigg((F_++F_-)G_+G_-+\left(\frac{G_+^2-G_-^2}{2G_+G_-}-(F_++F_-)^2G_+G_-\right)\frac{t}{u}\\
&\qquad\qquad+\left(\frac{F_+G_-^2-F_-G_+^2}{G_+G_-}+2F_+F_-(F_++F_-)G_+G_-\right)\frac{t^2}{u^2}\Bigg)\\
&\quad+(F_++F_-)G_+G_-\left(G_+G_--(F_++F_-)G_+G_-\frac{t}{u}+2F_+F_-G_+G_-\frac{t^2}{u^2}\right)\\
&=-\frac{G_+^2-G_-^2}{2}\cdot\frac{t}{u}+(-F_+G_-^2+F_-G_+^2)\frac{t^2}{u^2}
\end{aligned}
$$

by Lemmas 2.9, 2.11, 2.15, 2.19, 2.20, and 2.22.

Now since Lemma 2.9 implies that

$$
-\frac{G_+^2-G_-^2}{2}\cdot\frac{t}{u}=-\sum_{\substack{n\geq 0\\ n\,\mathrm{odd}}}\frac{2^{n+1}\pi^{2n}}{(2n+2)!}u^{2n-1}t=-\sum_{n\geq 0}\frac{2^{2n+2}\pi^{4n+2}}{(4n+4)!}u^{4n+1}t
$$

and that

$$
\begin{aligned}
&(-F_+G_-^2+F_-G_+^2)\frac{t^2}{u^2}\\
&\qquad=-\Big(\sum_{n_1\geq 0}2^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_0\geq 0}\frac{(-1)^{n_0}2^{n_0+1}\pi^{2n_0}}{(2n_0+2)!}u^{2n_0}\Big)\frac{t^2}{u^2}\\
&\qquad\quad+\Big(\sum_{n_1\geq 0}(-2)^{-n_1}\zeta(2n_1+1)u^{2n_1+1}\Big)\Big(\sum_{n_0\geq 0}\frac{2^{n_0+1}\pi^{2n_0}}{(2n_0+2)!}u^{2n_0}\Big)\frac{t^2}{u^2}
\end{aligned}
$$

$$= \sum_{n_0,n_1\ge 0} \frac{(-(-1)^{n_0}+(-1)^{n_1})2^{n_0-n_1+1}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)u^{2(n_0+n_1)-1}t^2$$
$$= \sum_{\substack{n_0,n_1\ge 0\\ n_0+n_1 \text{ odd}}} \frac{(-1)^{n_1}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)u^{2(n_0+n_1)-1}t^2,$$

we have

$$(-1)^n\zeta_{\mathcal{S}_3}(\{1,3\}^n,1)$$
$$= -\frac{2^{2n+2}\pi^{4n+2}}{(4n+4)!}t + \sum_{\substack{n_0,n_1\ge 0\\ n_0+n_1=2n+1}} \frac{(-1)^{n_1}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)t^2,$$

from which the theorem follows. ∎

2.6. Proof of Theorem 1.1. We define $\mathbb{Q}$-linear maps $I_0, I_1\colon \mathcal{I}\to\mathcal{I}$ by

$$I_0(k_1,\dots,k_r) = \sum_{i=0}^{r}(-1)^{k_{i+1}+\dots+k_r}(k_1,\dots,k_i)*(k_r,\dots,k_{i+1}),$$
$$I_1(k_1,\dots,k_r) = \sum_{i=0}^{r}(-1)^{k_{i+1}+\dots+k_r}(k_1,\dots,k_i)*\sigma(k_r,\dots,k_{i+1})$$

for all indices $(k_1,\dots,k_r)$, where $\sigma\colon\mathcal{I}\to\mathcal{I}$ is the $\mathbb{Q}$-linear map defined by

$$\sigma(k_1,\dots,k_r) = \sum_{\substack{l_1,\dots,l_r\ge 0\\ l_1+\dots+l_r=1}}(k_1+l_1,\dots,k_r+l_r)\prod_{i=1}^{r}\binom{k_i+l_i-1}{l_i}$$
$$= \sum_{i=1}^{r} k_i(k_1,\dots,k_{i-1},k_i+1,k_{i+1},\dots,k_r).$$

Observe that

$$\zeta^*_{\mathcal{S}_2}(k_1,\dots,k_r) = \zeta^*(I_0(k_1,\dots,k_r)) + \zeta^*(I_1(k_1,\dots,k_r))t.$$

Lemma 2.23. *If $\boldsymbol{k},\boldsymbol{l}\in\mathcal{I}$, then*

$$\sigma(\boldsymbol{k}*\boldsymbol{l}) = \sigma(\boldsymbol{k})*\boldsymbol{l}+\boldsymbol{k}*\sigma(\boldsymbol{l}).$$

Proof. We may assume that $\boldsymbol{k}$ and $\boldsymbol{l}$ are indices. We will prove the lemma by induction on the sum of the lengths of the indices. If either $\boldsymbol{k}$ or $\boldsymbol{l}$ is empty, then the assertion is obvious because $\sigma(\emptyset)=0$. If $\boldsymbol{k}$ and $\boldsymbol{l}$ are indices and k and l are positive integers such that

$$\sigma(\boldsymbol{k}*(\boldsymbol{l},l)) = \sigma(\boldsymbol{k})*(\boldsymbol{l},l)+\boldsymbol{k}*\sigma(\boldsymbol{l},l),$$
$$\sigma(\boldsymbol{k}*\boldsymbol{l}) = \sigma(\boldsymbol{k})*\boldsymbol{l}+\boldsymbol{k}*\sigma(\boldsymbol{l}),$$
$$\sigma((\boldsymbol{k},k)*\boldsymbol{l}) = \sigma(\boldsymbol{k},k)*\boldsymbol{l}+(\boldsymbol{k},k)*\sigma(\boldsymbol{l})$$

all hold, then

$$\sigma((\boldsymbol{k},k)*(\boldsymbol{l},l))=\sigma(\boldsymbol{k},k)*(\boldsymbol{l},l)+(\boldsymbol{k},k)*\sigma(\boldsymbol{l},l)$$

because

$$\begin{aligned}
&\sigma(\boldsymbol{k},k)*(\boldsymbol{l},l)+(\boldsymbol{k},k)*\sigma(\boldsymbol{l},l)\\
&=\big((\sigma(\boldsymbol{k}),k)+k(\boldsymbol{k},k+1)\big)*(\boldsymbol{l},l)+(\boldsymbol{k},k)*\big((\sigma(\boldsymbol{l}),l)+l(\boldsymbol{l},l+1)\big)\\
&\hspace{25em}\text{(definition of }\sigma)\\
&=(\sigma(\boldsymbol{k})*(\boldsymbol{l},l),k)+(\sigma(\boldsymbol{k})*\boldsymbol{l},k+l)+\big((\sigma(\boldsymbol{k}),k)*\boldsymbol{l},l\big)\\
&\quad+k(\boldsymbol{k}*(\boldsymbol{l},l),k+1)+k(\boldsymbol{k}*\boldsymbol{l},k+l+1)+k((\boldsymbol{k},k+1)*\boldsymbol{l},l)\\
&\quad+\big(\boldsymbol{k}*(\sigma(\boldsymbol{l}),l),k\big)+(\boldsymbol{k}*\sigma(\boldsymbol{l}),k+l)+((\boldsymbol{k},k)*\sigma(\boldsymbol{l}),l)\\
&\quad+l(\boldsymbol{k}*(\boldsymbol{l},l+1),k)+l(\boldsymbol{k}*\boldsymbol{l},k+l+1)+l((\boldsymbol{k},k)*\boldsymbol{l},l+1)\quad\text{(definition of }*)\\
&=(\sigma(\boldsymbol{k})*(\boldsymbol{l},l),k)+(\boldsymbol{k}*\sigma(\boldsymbol{l},l),k)+k(\boldsymbol{k}*(\boldsymbol{l},l),k+1)\\
&\quad+(\sigma(\boldsymbol{k})*\boldsymbol{l},k+l)+(\boldsymbol{k}*\sigma(\boldsymbol{l}),k+l)+(k+l)(\boldsymbol{k}*\boldsymbol{l},k+l+1)\\
&\quad+(\sigma(\boldsymbol{k},k)*\boldsymbol{l},l)+((\boldsymbol{k},k)*\sigma(\boldsymbol{l}),l)+l((\boldsymbol{k},k)*\boldsymbol{l},l+1)\quad\text{(definition of }\sigma)\\
&=\big(\sigma(\boldsymbol{k}*(\boldsymbol{l},l)),k\big)+k(\boldsymbol{k}*(\boldsymbol{l},l),k+1)\\
&\quad+(\sigma(\boldsymbol{k}*\boldsymbol{l}),k+l)+(k+l)(\boldsymbol{k}*\boldsymbol{l},k+l+1)\\
&\quad+\big(\sigma((\boldsymbol{k},k)*\boldsymbol{l}),l\big)+l((\boldsymbol{k},k)*\boldsymbol{l},l+1)\quad\text{(induction hypothesis)}\\
&=\sigma(\boldsymbol{k}*(\boldsymbol{l},l),k)+\sigma(\boldsymbol{k}*\boldsymbol{l},k+l)+\sigma((\boldsymbol{k},k)*\boldsymbol{l},l)\quad\text{(definition of }\sigma)\\
&=\sigma((\boldsymbol{k},k)*(\boldsymbol{l},l))\quad\text{(definition of }*).\ \blacksquare
\end{aligned}$$

LEMMA 2.24. *If a and b are odd positive integers, then*

$$I_0(\{a,b\}^n)=(-1)^n(\{a+b\}^n)$$

for every nonnegative integer n.

Proof. We proceed by induction on n. The assertion is obvious for $n=0$. Suppose that it is true for n. Write $k_i=a$ for odd i and $k_i=b$ for even i, so that $(k_1,\dots,k_{2n+2})=(\{a,b\}^{n+1})$. Then

$$\begin{aligned}
I_0(\{a,b\}^{n+1})&=I_0(k_1,\dots,k_{2n+2})\\
&=\sum_{i=0}^{2n+2}(-1)^{k_{i+1}+\cdots+k_{2n+2}}(k_1,\dots,k_i)*(k_{2n+2},\dots,k_{i+1})\\
&=\sum_{i=0}^{2n+2}(-1)^{i}(k_1,\dots,k_i)*(k_{2n+2},\dots,k_{i+1})\\
&=\sum_{i=1}^{2n+1}(-1)^{i}\big(((k_1,\dots,k_{i-1})*(k_{2n+2},\dots,k_{i+1}),k_i)\\
&\hspace{8em}+((k_1,\dots,k_i)*(k_{2n+2},\dots,k_{i+2}),k_{i+1})\big)
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{i=1}^{2n+1}(-1)^i((k_1,\dots,k_{i-1})*(k_{2n+2},\dots,k_{i+2}),k_i+k_{i+1})\\
&+(k_{2n+2},\dots,k_1)+(k_1,\dots,k_{2n+2})\\
&=\sum_{i=1}^{2n+1}(-1)^i((k_1,\dots,k_{i-1})*(k_{2n+2},\dots,k_{i+2}),k_i+k_{i+1})\\
&=-\Big(\sum_{i=0}^{2n}(-1)^i(k_1,\dots,k_i)*(k_{2n},\dots,k_{i+1}),a+b\Big)\\
&=-(I_0(k_1,\dots,k_{2n}),a+b)\\
&=-(I_0(\{a,b\}^n),a+b)\\
&=-(-1)^n(\{a+b\}^n,a+b) \quad \text{(induction hypothesis)}\\
&=(-1)^{n+1}(\{a+b\}^{n+1}). \ \blacksquare
\end{aligned}
$$

LEMMA 2.25. *If $k_1,\dots,k_r$ are positive integers with $k_1+\cdots+k_r$ even, then*

$$I_1(k_1,\dots,k_r)+I_1(k_r,\dots,k_1)=\sigma(I_0(k_1,\dots,k_r)).$$

Proof. We have

$$
\begin{aligned}
&I_1(k_1,\dots,k_r)+I_1(k_r,\dots,k_1)\\
&\quad=\sum_{i=0}^{r}(-1)^{k_{i+1}+\cdots+k_r}(k_1,\dots,k_i)*\sigma(k_r,\dots,k_{i+1})\\
&\qquad+\sum_{i=0}^{r}(-1)^{k_1+\cdots+k_i}(k_r,\dots,k_{i+1})*\sigma(k_1,\dots,k_i)\\
&\quad=\sum_{i=0}^{r}(-1)^{k_{i+1}+\cdots+k_r}\big((k_1,\dots,k_i)*\sigma(k_r,\dots,k_{i+1})\\
&\qquad\qquad+\sigma(k_1,\dots,k_i)*(k_r,\dots,k_{i+1})\big)\\
&\quad=\sum_{i=0}^{r}(-1)^{k_{i+1}+\cdots+k_r}\sigma((k_1,\dots,k_i)*(k_r,\dots,k_{i+1})) \quad \text{(Lemma 2.23)}\\
&\quad=\sigma(I_0(k_1,\dots,k_r)). \ \blacksquare
\end{aligned}
$$

LEMMA 2.26. *We have*

$$I_1(\{1,3\}^n)+I_1(\{3,1\}^n)=4(-1)^n\sum_{i=0}^{n-1}(-1)^i(4i+5)*(\{4\}^{n-i-1})$$

for every positive integer n.

Proof. We have

$$\begin{aligned}
&I_1(\{1,3\}^n)+I_1(\{3,1\}^n)\\
&\qquad=\sigma(I_0(\{1,3\}^n))\quad\text{(Lemma 2.25)}\\
&\qquad=(-1)^n\sigma(\{4\}^n)\quad\text{(Lemma 2.24)}\\
&\qquad=\binom{4+1-1}{1}(-1)^n((\{4\}^{n-1})\,\widetilde{ш}\,(5))\\
&\qquad=4(-1)^n\sum_{i=0}^{n-1}(-1)^i(4i+5)*(\{4\}^{n-i-1})\quad\text{(Lemma 2.16).}\ \blacksquare
\end{aligned}$$

Proof of Theorem 1.1. Lemma 2.24 shows that

$$\zeta_{\mathcal{S}_1}(\{1,3\}^n)=\zeta^*(I_0(\{1,3\}^n))=(-1)^n\zeta(\{4\}^n)=\frac{2(-4)^n}{(4n+2)!}\pi^{4n}$$

for every nonnegative integer n.

We now compute $\zeta(I_1(\{1,3\}^n))$, the coefficient of t in $\zeta_{\mathcal{S}_2}(\{1,3\}^n)$, for nonnegative integers n. Since obviously $\zeta(I_1(\{1,3\}^0))=0$, we assume $n\geq 1$. Lemma 2.26 shows that

$$\begin{aligned}
\zeta(I_1(\{1,3\}^n))+\zeta(I_1(\{3,1\}^n))&=4(-1)^n\sum_{i=0}^{n-1}(-1)^i\zeta(4i+5)\zeta(\{4\}^{n-i-1})\\
&=-4\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=n}}(-1)^{n_0}\zeta(\{4\}^{n_0})\zeta(4n_1+1)\\
&=-4\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=n}}\frac{2(-4)^{n_0}}{(4n_0+2)!}\pi^{4n_0}\zeta(4n_1+1).
\end{aligned}$$

Since Theorem 1.3 shows that

$$\begin{aligned}
\zeta(I_1(\{3,1\}^n))&=(-1)^{n+1}\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n}}\frac{(-1)^{n_0}2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\\
&=-(-1)^n\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n\\ n_0,n_1\text{ even}}}\frac{2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\\
&\quad+(-1)^n\sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n\\ n_0,n_1\text{ odd}}}\frac{2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)
\end{aligned}$$

$$
\begin{aligned}
&= -(-1)^n \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=n}} \frac{2^{2n_0-2n_1+2}}{(4n_0+2)!}\pi^{4n_0}\zeta(4n_1+1)\\
&\quad + (-1)^n \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n\\ n_0,n_1 \text{ odd}}} \frac{2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1),
\end{aligned}
$$

we obtain

$$
\begin{aligned}
\zeta(I_1(\{1,3\}^n)) &= -4 \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=n}} \frac{2(-4)^{n_0}}{(4n_0+2)!}\pi^{4n_0}\zeta(4n_1+1)\\
&\quad + (-1)^n \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=n}} \frac{2^{2n_0-2n_1+2}}{(4n_0+2)!}\pi^{4n_0}\zeta(4n_1+1)\\
&\quad - (-1)^n \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n\\ n_0,n_1 \text{ odd}}} \frac{2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1)\\
&= \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=n}} \frac{(-4)^{n_0+1}(2-(-4)^{-n_1})}{(4n_0+2)!}\pi^{4n_0}\zeta(4n_1+1)\\
&\quad - (-1)^n \sum_{\substack{n_0,n_1\geq 0\\ n_0+n_1=2n\\ n_0,n_1 \text{ odd}}} \frac{2^{n_0-n_1+2}}{(2n_0+2)!}\pi^{2n_0}\zeta(2n_1+1),
\end{aligned}
$$

as required. ■

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References

[1] H. Bachmann and S. Charlton, *Generalized Jacobi–Trudi determinants and evaluations of Schur multiple zeta values*, Eur. J. Combin. 87 (2020), art. 103133, 15 pp.

[2] H. Bachmann and Y. Yamasaki, *Checkerboard style Schur multiple zeta values and odd single zeta values*, Math. Z. 290 (2018), 1173–1197.

[3] J. Blümlein, D. J. Broadhurst, and J. A. M. Vermaseren, *The multiple zeta value data mine*, Comput. Phys. Comm. 181 (2010), 582–625.

[4] J. M. Borwein, D. M. Bradley, D. J. Broadhurst, and P. Lisoněk, *Combinatorial aspects of multiple zeta values*, Electron. J. Combin. 5 (1998), art. R38, 12 pp.

[5] J. M. Borwein, D. M. Bradley, D. J. Broadhurst, and P. Lisoněk, *Special values of multiple polylogarithms*, Trans. Amer. Math. Soc. 353 (2001), 907–941.

[6] D. Bowman and D. M. Bradley, *Resolution of some open problems concerning multiple zeta evaluations of arbitrary depth*, Compos. Math. 139 (2003), 85–100.

[7] M. E. Hoffman, *The algebra of multiple harmonic series*, J. Algebra 194 (1997), 477–495.

[8] K. Ihara, M. Kaneko, and D. Zagier, *Derivation and double shuffle relations for multiple zeta values*, Compos. Math. 142 (2006), 307–338.

[9] D. Jarossay, *Adjoint cyclotomic multiple zeta values and cyclotomic multiple harmonic values*, arXiv:1412.5099v5 (2019).

[10] M. Kaneko, *An introduction to classical and finite multiple zeta values*, Publ. Math. Besançon Algèbre Théor. Nombres 2019, no. 1, 103–129.

[11] M. Kaneko and D. Zagier, *Finite multiple zeta values*, in preparation.

[12] H. Murahara, T. Onozuka, and S. Seki, *Bowman–Bradley type theorem for finite multiple zeta values in $\mathcal{A}_2$*, Osaka J. Math. 57 (2020), 647–653.

[13] M. Ono, K. Sakurada, and S. Seki, *A note on $\mathcal{F}_n$-multiple zeta values*, Comment. Math. Univ. St. Pauli 69 (2021), 51–74.

[14] M. Ono, S. Seki, and S. Yamamoto, *Truncated t-adic symmetric multiple zeta values and double shuffle relations*, Res. Number Theory 7 (2021), art. 15, 28 pp.

[15] C. Reutenauer, *Free Lie Algebras*, London Math. Soc. Monogr. (N.S.) 7, Clarendon Press, Oxford Univ. Press, 1993.

[16] J. Rosen, *The completed finite period map and Galois theory of supercongruences*, Int. Math. Res. Notices 2019, 7379–7405.

[17] S. Saito and N. Wakabayashi, *Bowman–Bradley type theorem for finite multiple zeta values*, Tohoku Math. J. (2) 68 (2016), 241–251.

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