RELATIONSHIP BETWEEN MULTIPLE ZETA VALUES OF DEPTHS 2 AND 3 AND PERIOD POLYNOMIALS

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Abstract. Using the theory of motivic multiple zeta values, we examine some combinatorial aspects of the relationship between multiple zeta values of depths 2 and 3 and period polynomials.

1. Introduction

The multiple zeta value is defined by

\[ \zeta(n_1, \ldots, n_r) = \sum_{0 < k_1 < \cdots < k_r} \frac{1}{k_1^{n_1} \cdots k_r^{n_r}}, \]

for integers \( n_1, \ldots, n_r \geq 1 \) and \( n_r \geq 2 \). The relationship between multiple zeta values and modular forms on \( SL_2(\mathbb{Z}) \) or its period polynomials has been established in many papers \([2, 11, 15, 17, 18, 19, 20, 26, 27, 28]\) for depth 2 and \([3, 6, 8, 9, 10, 12, 22]\) for general case. In the present paper, we will give various connections between multiple zeta values of depths 2 and 3 and period polynomials.

The results on depth 2 and on depth 3 lie in slightly different contexts. For depth 2 case, motivated by the work of Gangl, Kaneko and Zagier \([11]\), we give a direct connection between even period polynomials of cusp forms and linear relations among \( \zeta(odd, odd) \)'s (see Theorem 2.2). A similar connection for the case \( \zeta(odd, even) \), which was developed by the first author in \([17, 18]\), will be also described in our setting (see Theorems 2.4 and 2.5). In depth 3, we give some indirect connections between period polynomials and linear relations among \( \zeta(odd, odd, even) \), \( \zeta(odd, even, odd) \) and \( \zeta(even, odd, odd) \) (see Theorems 2.7, 2.8 and 2.9). These results can be viewed as a generalization of the results given for the case \( \zeta(odd, odd) \) by Baumard and Schneps \([2]\) and for the case \( \zeta(odd, even) \) by Zagier \([28]\).

We also develop explicit computations for the isomorphism \( \phi : H \rightarrow U \) between the space \( H \) of motivic multiple zeta values and a certain universal algebra \( U \) (see Theorem 3.1). The formula plays a crucial role in the proofs of main results. For the convenience of the reader we repeat, in Sections 3 and 4, the relevant material from \([5]\) without proofs, thus making our exposition self-contained.
2. Main results

2.1. Depth 2. In [11], Gangl, Kaneko and Zagier gave an explicit formula for $\mathbb{Q}$-linear relations among double zeta values corresponding to restricted even period polynomials. Let us denote by $W_{ev}^N$ the space of the restricted even period polynomials of degree $N - 2$ (see (3.2) for the definition). A consequence of [11, Theorem 3] is as follows (they use the reverse order $k_1 > k_2 > 0$ for double zeta values $\zeta(n_1, n_2)$).

Proposition 2.1. For any $p(x_1, x_2) \in W_{ev}^N$, we have the relation of the form

\begin{equation}
\sum_{n_1 + n_2 = N \atop n_1, n_2 \geq 3: \text{odd}} q_{n_1, n_2} \zeta(n_1, n_2) \equiv 0 \mod \mathbb{Q} \zeta(N),
\end{equation}

where the coefficients $q_{r, s} \in \mathbb{Q}$ are given by

$$p(x_1 + x_2, x_1) = \sum_{n_1 + n_2 = N} \binom{N - 2}{n_1 - 1} q_{n_1, n_2} x_1^{n_1 - 1} x_2^{n_2 - 1}.$$ 

For example, for the first restricted even period polynomial $x_1^2 x_2^2 (x_1^2 - x_2^2)^3 \in W_{12}^{ev}$, with Proposition 2.1 one obtains the relation of the form

$$28 \zeta(3, 9) + 150 \zeta(5, 7) + 168 \zeta(7, 5) = \frac{5197}{691} \zeta(12),$$

where the coefficient of $\zeta(12)$ is computed from [11, Theorem 3], Euler’s formula for $\zeta(2n)$ and the stuffle product formula $\zeta(n_1) \zeta(n_2) = \zeta(n_1, n_2) + \zeta(n_2, n_1) + \zeta(n_1 + n_2)$.

We remark that in the previous result the polynomial $x_1^{N-2} - x_2^{N-2}$ corresponding to the Eisenstein series of weight $N$ on $SL_2(\mathbb{Z})$ produces the restricted sum formula (see [11, Theorem 1]); for $N$ even

\begin{equation}
\sum_{1 \leq n < N - 1 \atop n \text{ odd}} \zeta(n, N - n) = \frac{1}{4} \zeta(N).
\end{equation}

Since, as is known as the Eichler-Shimura-Manin correspondence, the space $\mathbb{C}(x_1^{N-2} - x_2^{N-2}) \oplus (W_N^N \otimes \mathbb{C})$ is isomorphic to the space of modular forms of weight $N$ on $SL_2(\mathbb{Z})$, the above results lead to a correspondence between modular forms and linear relations among double zeta values.

Motivated by this work, we give a more elaborate correspondence between even period polynomials associated to cusp forms and linear relations among double zeta values, from which an explicit formula for the coefficient of $\zeta(N)$ in the relation (2.1) is obtained. Let $S_N$ denote the space of cusp forms of weight $N$ on $SL_2(\mathbb{Z})$. We define the even period polynomial $P_f^{ev}(x_1, x_2)$ of a cusp form $f \in S_N$ by

$$P_f^{ev}(x_1, x_2) := \sum_{n_1 + n_2 = N \atop n_1, n_2 \geq 1: \text{odd}} (-1)^{n_2 - 1} \binom{N - 2}{n_2 - 1} L_f(n_2) x_1^{n_1 - 1} x_2^{n_2 - 1}$$
where $L_f(s) = \int_0^\infty f(it)t^{s-1}dt$. This is the even polynomial part of the period polynomial $\int_0^\infty f(it)(x_1 - tx_2)^{k-2}dt$. Instead of double zeta values, we consider

$$\zeta^\sharp(n_1, n_2) = \zeta(n_1, n_2) + \frac{1}{2}\zeta(n_1 + n_2),$$

which is a special case of Yamamoto’s $t$-interpolated multiple zeta values with $t = \frac{1}{2}$ (see [24]). The first main result of this paper is as follows.

**Theorem 2.2.** For any $f \in S_N$, we define numbers $\{a_{n_1, n_2} \in \mathbb{C} \mid n_1 + n_2 = N\}$ by

$$P_f^\text{ev}(x_1 + x_2, x_1) = \sum_{n_1 + n_2 = N} \binom{N-2}{n_1-1} a_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1}.$$

Note that $a_{N-1, 1} = 0$. Then we have

$$\sum_{n_1 + n_2 = N \atop n_1 \geq 1 \text{ odd}} a_{n_1, n_2} \zeta^\sharp(n_1, n_2) = 0.$$

Since there is a basis $\{f_1\}$ of the space $S_N$ such that $P_{f_1}^\text{ev} \in \mathbb{Q}[x, y]$ (see [16]), the relation in Theorem 2.2 can be over $\mathbb{Q}$. The first example of even period polynomials is given for the cusp form $\Delta = q \prod_{n=1}^\infty (1 - q^n)^24$ of weight 12 by

$$c^{-1} P_{\Delta}^\text{ev}(x_1, x_2) = \frac{36}{691} (x_1^{10} - x_2^{10}) - x_1^2 x_2^2 (x_1^2 - x_2^2)^3,$$

where the constant $c$ is the coefficient of $x_1^3 x_2^5$ in $P_{\Delta}^\text{ev}(x_1, x_2)$. For this, normalizing coefficients, with Theorem 2.2 we obtain

$$22680 \zeta^\sharp(1, 11) + 13006 \zeta^\sharp(3, 9) - 29145 \zeta^\sharp(5, 7) - 35364 \zeta^\sharp(7, 5) + 22680 \zeta^\sharp(9, 3) = 0.$$

As an application of Theorem 2.2 one can give an explicit formula for the coefficient of $\zeta(N)$ in the relation (2.1).

**Corollary 2.3.** For any $f \in S_N$, we define numbers $\{q_{n_1, n_2} \in \mathbb{C} \mid n_1 + n_2 = N\}$ by

$$P_f^\text{ev,0}(x_1 + x_2, x_1) = \sum_{n_1 + n_2 = N} \binom{N-2}{n_1-1} q_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1},$$

where we set $P_f^\text{ev,0}(x_1, x_2) = P_f^\text{ev}(x_1, x_2) - L_f^\ast(1)(x_1^{N-2} - x_2^{N-2})$. Then we have

$$\sum_{n_1 + n_2 = N \atop n_1, n_2 \geq 3 \text{ odd}} q_{n_1, n_2} \zeta(n_1, n_2) = -\frac{1}{2} \left( \frac{N+1}{2} L_f^\ast(1) + \sum_{n_1 + n_2 = N \atop n_1, n_2 \geq 3 \text{ odd}} q_{n_1, n_2} \right) \zeta(N).$$

In [28] Section 6], Zagier also found a connection between modular forms and double zeta values of odd weight. For this, in [17] Theorems 1 and 2] the first author obtains a similar result to Proposition 2.1. On this occasion, we recast the statement with
For \( f \in S_N \), we denote the odd period polynomial of \( f \) by
\[
P_f^{\text{od}}(x_1, x_2) := \sum_{n_1 + n_2 = N, n_1, n_2 \geq 1, \text{odd}} (-1)^{n_2} \binom{N-2}{n_2-1} L^*_f(n_2)x_1^{n_1-1}x_2^{n_2-1}.
\]

**Theorem 2.4.** For any \( f \in S_N \), we define numbers \( \{b_{n_1, n_2} \in \mathbb{C} \mid n_1 + n_2 = N\} \) by
\[
P_f^{\text{od}}(x_1 + x_2, x_2) - \frac{x_1}{x_2} P_f^{\text{od}}(x_1 + x_2, x_1) = \sum_{n_1 + n_2 = N} \binom{N-1}{n_1-1} b_{n_1, n_2} x_1^{n_1-1}x_2^{n_2-1}.
\]
Then we have
\[
\sum_{n_1 + n_2 = N, n_1, n_2 \geq 1, \text{odd}} b_{n_1, n_2} \zeta^{\frac{1}{2}}(n_1, n_2 + 1) = 0.
\]

For example, for the odd period polynomial corresponding to \( \Delta \) given by
\[
(2.4) \quad 4x_1^2x_2 - 25x_1^7x_2^2 + 42x_1^5x_2^2 - 25x_1^3x_2^2 + 4x_1^9
\]
up to constant, using Theorem [2.3] and normalizing coefficients, one gets
\[-12\zeta^{\frac{1}{2}}(3, 10) - 14\zeta^{\frac{1}{2}}(5, 8) + 5\zeta^{\frac{1}{2}}(7, 6) + 18\zeta^{\frac{1}{2}}(9, 3) = 0.
\]

**Theorem 2.5.** For any \( f \in S_N \), we define numbers \( \{c_{n_1, n_2} \in \mathbb{C} \mid n_1 + n_2 = N\} \) by
\[
\frac{d}{dx_1} P_f^{\text{ev}}(x_1 + x_2, x_2) - \frac{d}{dx_2} P_f^{\text{ev}}(x_1 + x_2, x_1) = \sum_{n_1 + n_2 = k-1} \binom{N-3}{n_1-1} c_{n_1, n_2} x_1^{n_1-1}x_2^{n_2-1}.
\]
Then we have
\[
\sum_{n_1 + n_2 = N-1, n_1 \geq 1, \text{odd}} c_{n_1, n_2} \zeta^{\frac{1}{2}}(n_1, n_2) = 0.
\]

For example, for the polynomial (2.3), by Theorem [2.5] and normalizing coefficients, we have
\[-14\zeta^{\frac{1}{2}}(3, 8) + 10\zeta^{\frac{1}{2}}(5, 6) - 21\zeta^{\frac{1}{2}}(7, 4) = 0.
\]

### 2.2. Depth 3

In depth 3, although we are not able to give explicit \( \mathbb{Q} \)-linear relations corresponding to period polynomials, its dual counterpart is derived. As a prototype, we have in mind the analogues story for works on \( \zeta(\text{odd, odd}) \) by Baumard and Schneps [2] and on \( \zeta(\text{odd, even}) \) by Zagier [28, Section 6]. Making use of the double shuffle Lie algebra, Baumard and Schneps [2] introduced the matrix \( C_N \) (we use a slightly different definition in (2.4)). The matrix \( C_N \) characterizes the relation (2.1) and the relation among elements in the double shuffle Lie algebra of depth 2 (the Ihara-Takao relation). Their results are summarized as follows.

**Proposition 2.6.**

(i) All right annihilator of the matrix \( C_N \) gives the relation of the form (2.1).
(ii) The spaces \( W_N^{\text{ev}} \) and \( \ker C_N \) are canonically isomorphic to each other, where \( \ker C_N \) denotes the space of left annihilators of the matrix \( C_N \).

For this, they showed in [2, Theorem 3.1] that both results on the left and right annihilators are deduced from each other by duality. Likewise, Zagier [28] introduced the matrix \( B_N \) (see (8.1)) and showed that all right annihilators of the matrix \( B_N \) produce \( \mathbb{Q} \)-linear relations among \( \zeta(\text{odd, even})'s \) and that there is the injective map \( W_{N+1}^{\text{ev}} \oplus W_{N-1}^{\text{odd}} \to \ker B_N \), where \( W_N^{\text{odd}} \) denotes the space of odd period polynomials of degree \( N - 2 \) (see (33) for the definition). We will recall these results, which are needed in the proofs of our second main results.

Our results slightly generalize the above results to the case for \( j \)-th almost totally odd triple zeta values \( \zeta(\text{odd, odd, even}, \zeta(\text{odd, even, odd}) \) and \( \zeta(\text{even, odd, odd}) \), where \( j \) indicates the position of \( \text{even} \) (see Definition 6.1). For this, we shall use the theory of motivic multiple zeta values to introduce the matrix \( C_N^{(j)} \) for each \( j \)-th almost totally odd triple zeta values (see Definition 6.3). As a generalization of Proposition 2.6 (i), we will see that all right annihilator of the matrix \( C_N^{(j)} \) gives \( \mathbb{Q} \)-linear relations among \( j \)-th almost totally odd motivic triple zeta values, and vice versa (see Theorem 6.4).

In contrast with Proposition 2.6 (ii), our results on left annihilators provide various connections with period polynomials. We first state the connection between \( \ker C_N^{(j)} \) (the space of left annihilators) and restricted even period polynomials for each \( j = 1, 2, 3 \). In the case \( j = 3 \), the space \( \ker C_N^{(3)} \) has more connections with restricted even and odd period polynomials, which is then described.

Let \( P_N^{\text{ev}} \) be the \( \mathbb{Q} \)-vector space spanned by the polynomials
\[
p(x_1, x_2)x_3^{N-k-1} \quad (p(x_1, x_2) \in W_k^{\text{ev}}, 0 < k < N).
\]
It follows from the definition that for \( N > 0 \) even one has
\[
P_N^{\text{ev}} \cong \bigoplus_{1 < k < N \atop k \text{ even}} (W_k^{\text{ev}} \otimes \mathbb{Q}x_3^{N-k-1}).
\]
Note that the first example of elements in \( P_N^{\text{ev}} \) is in \( N = 14 \); it is \((x_1^8x_2^8 - 3x_1^4x_2^6 + 3x_1^6x_2^4 - x_1^3x_2^5)x_3 \in P_3^{\text{ev}} \). Let
\[
\Pi_N^{(3)} = \{ n = (n_1, n_2, n_3) \in \mathbb{Z}_{>1}^3 \mid n_1 + n_2 + n_3 = N, n_1, n_2 : \text{odd}, n_3 : \text{even} \},
\]
and denote by \( (a_n)_{n \in \Pi_N^{(3)}} \) a row vector in \( \ker C_N^{(j)} \), namely, \( (a_n)_{n \in \Pi_N^{(3)}} \cdot C_N^{(j)} = 0 \), the zero vector. With this notation, we have the following result.

**Theorem 2.7.** For \( j = 1, 2, 3 \) and \( N > 0 \) even, the map
\[
P_N^{\text{ev}} \to \ker C_N^{(j)}
\]
\[
\sum_{n \in \Pi_N^{(3)}} a_n x^n \mapsto (a_n)_{n \in \Pi_N^{(3)}}
\]
is well-defined and injective, where we write \( x^n = x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1} \) for \( n = (n_1, n_2, n_3) \).

For example, it can be checked that the row vector
\[
(-1 \ 3 \ -3 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0)
\]
corresponding to the element of \( \mathbb{P}_{14}^{ev} \) is a left annihilator of the matrix \( C_{14}^{(2)} \) (see (6.5)).

In the case \( j = 3 \), one can naturally decompose the matrix \( C_N^{(3)} \) into the square matrices \( B_N^{(3)} \) and \( E_N^{(3)} \), namely \( C_N^{(3)} = B_N^{(3)}E_N^{(3)} \). Then, by linear algebra, we have
\[
\ker C_N^{(3)} = \ker B_N^{(3)} \oplus (\text{Im } B_N^{(3)} \cap \ker E_N^{(3)}),
\]
where the matrix is viewed as a map on the vector spaces (see Section 6.2 for the details). We now describe a connection between period polynomials and \( B_N^{(3)} \) and \( \text{Im } B_N^{(3)} \cap \ker E_N^{(3)} \), separately.

For \( \ker B_N^{(3)} \), we define the subspace \( Q_N^{ev} \subset \mathbb{Q}[x_1, x_2, x_3] \) (resp. \( Q_N^{od} \subset \mathbb{Q}[x_1, x_2, x_3] \)) as the \( \mathbb{Q} \)-vector space spanned by \( x_1^{k-1}p(x_2, x_3) \) for \( p(x_1, x_2) \in \mathbb{W}_{N-k+1}^{ev} \) and \( 1 < k < N \) odd (resp. \( x_1^{k-1}p(x_2, x_3) \) for \( p(x_1, x_2) \in \mathbb{W}_{N-k+1}^{od} \) and \( 1 < k < N \) odd), namely, for \( N \) even
\[
Q_N^{ev} \cong \bigoplus_{1 < k < N \atop k \text{ odd}} (\mathbb{Q}x^k \otimes \mathbb{W}_{N-k+1}^{ev}),
\]
\[
Q_N^{od} \cong \bigoplus_{1 < k < N \atop k \text{ odd}} (\mathbb{Q}x^k \otimes \mathbb{W}_{N-k+1}^{od})
\]
holds. For simplicity of notation, for any subsets \( S_1, \ldots, S_r \) of \( \mathbb{Z} \), we let
\[
\mathbb{I}_N(S_1, \ldots, S_r) = \{(n_1, \ldots, n_r) \in S_1 \times \cdots \times S_r \mid N = n_1 + \cdots + n_r \}.
\]
We denote by \( o \) (resp. \( e \)) the set of all odd integers \( > 1 \) (resp. all even integers \( > 1 \)).

For example, it follows that \( \mathbb{I}_N^{(3)} = \mathbb{I}_N(oee) \).

**Theorem 2.8.** The maps
\[
\sum_{n \in \mathbb{I}_{N+1}^{(3)}(oo)} a_n x^n \mapsto (a_n^+)_{n \in \mathbb{I}_N^{(3)}} \quad \text{and} \quad \sum_{n \in \mathbb{I}_{N-1}^{(3)}(oe)} a_n x^n \mapsto (a_n^-)_{n \in \mathbb{I}_N^{(3)}}
\]
are well-defined and injective, where \( a_n^+ = n_3a_{n_1,n_3+1,n_2} \) and \( a_n^- = a_{n_1,n_2-1,n_3} \) for \( n = (n_1, n_2, n_3) \). Furthermore, their combined map \( Q_N^{ev} \oplus Q_N^{od} \to \ker B_N^{(3)} \) is an injection.

For \( \text{Im } B_N^{(3)} \cap \ker E_N^{(3)} \), we define the subspace \( \mathbb{P}_N^{ev} \subset \mathbb{Q}[x_1, x_2, x_3^{N-1}] \) as the \( \mathbb{Q} \)-vector space spanned by \( p(x_1, x_2)x_3^{N-k-1} \) for \( p(x_1, x_2) \in \mathbb{W}_k^{ev} \) and \( 0 < k \leq N \) even, namely, for \( N \) even we have
\[
\mathbb{P}_N^{ev} \cong \bigoplus_{0 < k \leq N \atop k \text{ even}} (\mathbb{W}_k^{ev} \otimes \mathbb{Q}x_3^{N-k-1}).
\]
Theorem 2.9. There is a well-defined linear map from $\hat{\mathcal{P}}_N$ to $\text{Im} B_N^{(3)} \cap \ker E_N^{(3)}$.

Since the matrix $C_N^{(j)}$ is a $|\mathbb{N}_N| \times |\mathbb{N}_N|$ matrix, we see by Theorem 6.4 that a lower bound of $\dim \ker C_N^{(j)}$ gives an upper bound of the dimension of the $\mathbb{Q}$-vector space spanned by all $j$-th almost totally odd triple zeta values of weight $N$. Our results therefore provide an application to give an upper bound of the dimension. Let us consider the lower bound of $\dim \ker C_N^{(j)}$ obtained by our results. Before this, we give a predicted number of $\dim \ker C_N^{(j)}$. Let

$$\mathcal{O}(x) = \frac{x^3}{1 - x^2} = x^3 + x^5 + \cdots, \quad \mathcal{E}(x) = \frac{x^2}{1 - x^2} = x^2 + x^4 + \cdots$$

and set

$$\mathcal{S}(x) = \frac{x^{12}}{(1 - x^4)(1 - x^6)} = \sum_{N>0} \dim S_N x^N.$$

Using Mathematica we have checked the following equality up to $N = 40$.

Conjecture 2.10. We have

$$\sum_{N>0} \dim_\mathbb{Q} \ker C_N^{(1)} x^N \stackrel{?}{=} \frac{1}{x^2} \mathcal{S}(x) \mathcal{E}(x),$$

$$\sum_{N>0} \dim_\mathbb{Q} \ker C_N^{(2)} x^N \stackrel{?}{=} \mathcal{S}(x) \mathcal{E}(x),$$

$$\sum_{N>0} \dim_\mathbb{Q} \ker C_N^{(3)} x^N \stackrel{?}{=} \frac{1}{x^2} \mathcal{S}(x) \mathcal{E}(x) + \left( x + \frac{1}{x} \right) \mathcal{S}(x) \mathcal{O}(x).$$

By (3.4), it can be shown that

$$\sum_{N>0} \dim_\mathbb{P}_N^{ev} x^N = \mathcal{S}(x) \mathcal{E}(x), \quad \sum_{N>0} \dim_\mathbb{Q}_N^{ev} x^N = \frac{1}{x} \mathcal{S}(x) \mathcal{O}(x),$$

$$\sum_{N>0} \dim_\mathbb{Q}_N^{od} x^N = x \mathcal{S}(x) \mathcal{O}(x), \quad \sum_{N>0} \dim_\mathbb{P}_N^{ev} x^N = \frac{1}{x^2} \mathcal{S}(x) \mathcal{E}(x).$$

With this, it follows easily that Theorem 2.7 gives the best lower bound of $\dim \ker C_N^{(2)}$ (note that this lower bound also follows from the result of Goncharov [12]). We also see that Theorems 2.8 and 2.9 seem to give the best lower bound of $\dim \ker C_N^{(3)}$ (assuming the injectivity of the map in Theorem 2.9, we get the best lower bound; see Remark 8.4). According to Conjecture 2.10, we should have more elements in $\ker C_N^{(1)}$ which does not come from Theorem 2.7. We are expecting that they are obtained from the derivative of odd period polynomial (see Remark 7.3). This could be an interesting phenomena since this is the first appearance of the derivative of odd period polynomial in this study.
As an application of our study on the matrices $C^{(j)}_N$, one can deduce an explicit formula for the parity theorem for $j$-th almost totally odd triple zeta values, which will be described in the last section (Theorem 9.1).

2.3. Contents of the paper. In Section 3, we prepare some notations and fundamental properties of period polynomials and motivic multiple zeta values. The goal for the motivic multiple zeta value is to describe the isomorphism $\phi : H \to U$. We develop explicit formulas for $\phi(\zeta^m(n_1, n_2))$ and $\phi(\zeta^m(n_1, n_2, n_3))$ (Proposition 4.6, Theorem 4.7 and Proposition 4.10) in Section 4. Section 5 is devoted to a proof of Theorem 2.2. In the proof, we will see that the rational solution to the double shuffle equation (4.4) of depth 2 is orthogonal to the extra relation among periods of a cusp form given by Kohnen and Zagier [16, Theorem 9]. In Section 6, we give some background of $j$-th almost totally odd multiple zeta values and discuss the matrix $C^{(j)}_N$. In Section 7, we will prove Theorem 2.7. In Section 8, we will show Theorem 2.8 and 2.9. Finally, as an application of our study of the matrix $C^{(j)}_N$, we give an explicit formula for the parity theorem of $j$-th almost totally odd triple zeta values in Section 9.

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3. Preliminaries

3.1. Fundamental of period polynomials. Let $V_N$ denotes the $\mathbb{Q}$-vector space of homogenous polynomials of degree $N - 2$:

$$V_N = \bigoplus_{0 < n < N} \mathbb{Q}x_1^{n-1}x_2^{N-n-1}.$$ 

We write $V_N^\mathbb{C} = V_N \otimes_{\mathbb{Q}} \mathbb{C}$. The action of the group $\Gamma = \text{PGL}_2(\mathbb{Z})$ is defined in the standard manner by $(p|\gamma)(x_1, x_2) = p(ax_1 + bx_2, cx_1 + dx_2)$ for $\gamma = \left( \begin{smallmatrix} a & b \\ c & d \end{smallmatrix} \right) \in \Gamma$ and $p \in V_N$. Following [13], we let

$$(3.1) \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad U = TS, \quad \varepsilon = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \delta = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$ 

With this, we denote by

$$(3.2) \quad W_N^\mathbb{C} = \{ p \in V_N \mid p|(1 - T + T\varepsilon) = 0 \}$$
the \( \mathbb{Q} \)-vector space of restricted even period polynomials of degree \( N - 2 \), where we have extended the action of \( \Gamma \) to its group ring by linearity. We also denote by
\[
W^\text{ev}_N = \{ p \in V_N \mid p | (1 - T - T \varepsilon) = 0 \}
\]
the \( \mathbb{Q} \)-vector space of odd period polynomials of degree \( N - 2 \). We note that for any \( f \in S_N \) we have
\[
P_{f}^{\text{ev}, 0}(x_1, x_2) \in W^\text{ev}_N \otimes \mathbb{Q} \mathbb{C}, \quad P_{f}^{\text{od}}(x_1, x_2) \in W^\text{od}_N \otimes \mathbb{Q} \mathbb{C},
\]
where \( P_{f}^{\text{ev}, 0}(x_1, x_2) = P_{f}^{\text{ev}}(x_1, x_2) - L_{f}^{*}(1)(x_1^{N-2} - x_2^{N-2}) \). An important fact about these polynomials is that the dimension of \( W^\text{ev}_N \) and \( W^\text{od}_N \) equals the dimension of the space of cusp forms of weight \( N \) for \( \text{SL}_2(\mathbb{Z}) \):
\[
\sum_{N > 0} \dim_{\mathbb{Q}} W^\text{ev}_N x^N = \sum_{N > 0} \dim_{\mathbb{Q}} W^\text{od}_N x^N = S(x),
\]
which is known as Eichler–Shimura–Manin correspondence (see [16, Section 1.1] and see also [2, Section 1.1] for the space \( W^\text{ev}_N \)).

3.2. Motivic multiple zeta values. We follow the notation of [5]. The definition of the motivic multiple zeta value \( \zeta^m(n_1, \ldots, n_r) \) we use is referred to [5, Definition 2.1], where \( \zeta^m(2) \) is not treated to be zero. A more elaborate definition can be found in [7, Section 2.2] where the motivic multiple zeta value is defined as a motivic period of the Tannakian category of the mixed Tate motives over \( \mathbb{Z} \).

Let \( \mathcal{H} \) be the \( \mathbb{Q} \)-vector space spanned by all motivic multiple zeta values. As usual, we call \( n_1 + \cdots + n_r \) the weight and \( r \) the depth for \( \zeta^m(n_1, \ldots, n_r) \). The space \( \mathcal{H} \) has the structure of a graded \( \mathbb{Q} \)-algebra:
\[
\mathcal{H} = \bigoplus_{N \geq 0} \mathcal{H}_N,
\]
where \( \mathcal{H}_N \) denotes the \( \mathbb{Q} \)-vector space spanned by all motivic multiple zeta values of weight \( N \). We regard \( 1 \in \mathbb{Q} \) as the unique motivic multiple zeta value of weight 0 and depth 0. The product on \( \mathcal{H} \) is naturally given by the shuffle product of iterated integrals (see (3.6) below). There is the period map from the space \( \mathcal{H} \) to \( \mathbb{R} \) sending the motivic multiple zeta value \( \zeta^m(n_1, \ldots, n_r) \) to the real number \( \zeta(n_1, \ldots, n_r) \) (see (1.1)), or rather, the regularised multiple zeta value with respect to the shuffle product.

3.3. Motivic iterated integrals. For \( a_i \in \{0, 1\} \) we denote by
\[
I^m(a_0; a_1, \ldots, a_N; a_{N+1}) \in \mathcal{H}_N
\]
the motivic iterated integral (see [5, (2.16)]), which is defined by extending Goncharov’s motivic iterated integrals [12]. With this, the motivic multiple zeta value is given in
the following manner:

\[ \zeta^m(n_1, \ldots, n_r) = I^m(0; 1, 0, \ldots, 0, \underbrace{1, 0, \ldots, 0}_{n_1-1}, \ldots, 0, \underbrace{1, 0, \ldots, 0}_{n_r-1}). \]

Motivic iterated integrals satisfy the following relations (see \[5\] p.955):

- The unit is given by \( I^m(a; b) \) for \( a, b \in \{0, 1\} \).
- The product is given by the shuffle product: for all integers \( N, N' \geq 0 \) and \( a_1 \in \{0, 1\} \), one has

\[
I^m(a_0; a_1, \ldots, a_N; a_{N+N'+1}) = \sum_{\sigma \in \Sigma(N,N')} I^m(a_0; a_{\sigma^{-1}(1)}, \ldots, a_{\sigma^{-1}(N+N')}; a_{N+N'+1}),
\]

where \( \Sigma(N,N') \) is the set of \( \sigma \) in the symmetric group \( \mathfrak{S}_{N+N'} \) such that \( \sigma(1) < \cdots < \sigma(N) \) and \( \sigma(N+1) < \cdots < \sigma(N+N') \).
- For \( N \geq 1 \) and \( a, a \in \{0, 1\}, \) we have

\[
I^m(a; a_1, \ldots, a_N; a) = 0.
\]
- For any \( a_i \in \{0, 1\}, \) we have

\[
I^m(a_0; a_1, \ldots, a_N; a_{N+1}) = (-1)^N I^m(a_{N+1}; a_N, \ldots, a_1; a_0).
\]

We remark that the last identity (3.8) essentially follows from (3.6) and the path composition formula \[12\] (iii) p.224 satisfied by iterated integrals.

We further remark that for any \( a, b, c \in \{0, 1\}, \) since \( I^m(a; b; c) \in H_1 = \{0\}, \) it can be seen from (3.6) that

\[
0 = \frac{1}{n!} I^m(a; b; c)^n = I^m(a; b, \ldots, b; c) \quad (n \geq 1).
\]

3.4. **Coaction on the space \( \mathcal{H} \).** Let us denote by \( \mathcal{A} \) the quotient algebra \( \mathcal{H}/\zeta^m(2)\mathcal{H} \) and by \( I^a \) the image of an motivic iterated integral \( I^m \) in the space \( \mathcal{A} \):

\[ \mathcal{A} = \mathcal{H}/\zeta^m(2)\mathcal{H}. \]

Then the space \( \mathcal{H} \) forms a graded \( \mathcal{A} \)-comodule over \( \mathbb{Q} \) (see \[5\] Theorem 2.4) with the coaction

\[ \Delta : \mathcal{H} \longrightarrow \mathcal{A} \otimes \mathcal{H}. \]

The coaction \( \Delta \) is computed for the element (3.5) by the formula

\[
\sum_{0 \leq k \leq N} \sum_{i_0 < i_1 < \cdots < i_k < i_{k+1}} \left\{ \prod_{p=0}^{k} I^a(a_{i_p}; a_{i_{p+1}}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}}) \right\} \otimes I^m(a_0, a_{i_1}, \ldots, a_{i_k}; a_{N+1}),
\]

\[ (3.10) \]
which can be found in [5, Eq. (2.18)]. It is originally given by Goncharov (see [12, Eq. (27)]) with the factors interchanged. We note that the quotient space $\mathcal{A}$ carries a Hopf algebra structure with the product given by the shuffle product and the coproduct $\Delta : \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}$ induced by the coaction $\Delta$ on $\mathcal{H}$.

3.5. **Algebra comodule structure of the space $\mathcal{H}$**. Let $\mathcal{U}'$ be the noncommutative polynomial algebra freely generated by symbols $f_{2i+1}$ in weight $2i + 1$:

$$\mathcal{U}' = \mathbb{Q}\langle f_{2i+1} \mid i \geq 1 \rangle.$$ 

The vector space $\mathcal{U}'$ is equipped with the product given by the shuffle product in

$$f_{i_1} \cdots f_{i_r} \mathfrak{m} f_{i_{r+1}} \cdots f_{i_{r+s}} = \sum_{\sigma \in \Sigma(r,s)} f_{i_{\sigma^{-1}(1)}} \cdots f_{i_{\sigma^{-1}(r+s)}}$$

and the coproduct given by the deconcatenation $\Delta^*$

$$(3.11) \quad \Delta^*(f_{i_1} \cdots f_{i_r}) = \sum_{j=0}^{r} f_{i_1} \cdots f_{i_j} \otimes f_{i_{j+1}} \cdots f_{i_r}.$$ 

With this, the space $\mathcal{U}'$ carries a Hopf algebra structure, where the antipode $S$ (see [14, Proposition V.2.4.]) is given by the formula $S(f_{i_1} \cdots f_{i_r}) = (-1)^r f_{i_r} \cdots f_{i_1}$, which we do not use in this paper. We note that the Hopf algebra $\mathcal{U}'$ is isomorphic to the ring of regular functions on the unipotent radical of the motivic Galois group of the Tannakian category of the mixed Tate motives over $\mathbb{Z}$.

Let us consider the graded vector space

$$\mathcal{U} := \mathcal{U}' \otimes \mathbb{Q}[f_2] = \bigoplus_{N \geq 0} \mathcal{U}_N,$$

where $f_2$ is a commutative symbol of weight 2 and $\mathcal{U}_N$ denotes the graded weight $N$ part of $\mathcal{U}$. The space $\mathcal{U}$ carries a graded $\mathcal{U}'$-comodule structure, with the coaction $\Delta^* : \mathcal{U} \to \mathcal{U}' \otimes \mathcal{U}$ satisfying $\Delta^*(f_2) = 1 \otimes f_2$ and $\Delta^*(wf^k) = \Delta^*(w)\Delta^*(f_2)^k$ for any $k > 0$ and $w \in \mathcal{U}'$.

It was shown by Goncharov that there is a non-canonical embedding

$$\phi' : \mathcal{A} \to \mathcal{U}'$$

as Hopf algebras. Since we have $\mathcal{H} \cong \mathcal{A} \otimes \mathbb{Q}[\zeta^m(2)]$ and $\Delta(\zeta^m(2)) = 1 \otimes \zeta^m(2)$, the embedding $\phi'$ can be extended to the algebra comodule homomorphism $\phi : \mathcal{H} \to \mathcal{U}$, i.e. $\Delta^* \circ \phi = (\phi' \otimes \phi) \circ \Delta$ holds. By [5, Lemma 3.2], we can normalise the choice of embedding $\phi : \mathcal{H} \to \mathcal{U}$ as

$$\phi(\zeta^m(N)) = f_N$$

for $N \geq 2$, where we put

$$f_{2k} := \frac{\zeta^m(2k)}{\zeta^m(2)^k} f^k_2 \ (k \geq 1).$$
Since the Hoffman basis conjecture is true for motivic multiple zeta values [5, Theorem 1.1], we have the following theorem.

**Theorem 3.1.** There is a non-canonical isomorphism
\[ \phi : \mathcal{H} \rightarrow \mathcal{U} \]
as algebra comodules, sending \( \zeta^m(N) \) to \( f_N \) for \( N \geq 2 \).

Computing the image of the motivic multiple zeta value under the isomorphism \( \phi \) plays a crucial role in this paper. In the next section, we shall compute \( \phi(\zeta^m(n_1, n_2)) \) and \( \phi(\zeta^m(n_1, n_2, n_3)) \).

4. A computation of the isomorphism \( \phi \)

4.1. **The Brown operator** \( D_m \). Let \( \mathcal{L} := \mathcal{A}_{>0}/(\mathcal{A}_{>0})^2 \) be the tangent space of \( \mathcal{A} \), which is a Lie coalgebra, and \( \pi_m : \mathcal{A}_{>0} \rightarrow \mathcal{L}_m \) the natural projection taking the graded weight \( m \) part \( \mathcal{L}_m \) of the graded vector space \( \mathcal{L} = \bigoplus_{m > 0} \mathcal{L}_m \).

**Definition 4.1 (The Brown operator).** We define the linear map \( D_m \) for all odd integer \( m > 1 \) by the following composition map:
\[
D_m : \mathcal{H} \xrightarrow{\Delta - 1 \otimes \text{id}} \mathcal{A}_{>0} \otimes \mathcal{H} \xrightarrow{\pi_m \otimes \text{id}} \mathcal{L}_m \otimes \mathcal{H}.
\]

One can easily check that the map \( D_m \) is a derivation (i.e. \( D_m(\xi_1 \xi_2) = (1 \otimes \xi_1)D_m(\xi_2) + (1 \otimes \xi_2)D_m(\xi_1) \) for any \( \xi_1, \xi_2 \in \mathcal{H} \)). From (3.10), we find that the formula of the map \( D_m \) for the element (3.5) is given by
\[
(4.1) \quad \sum_{p=0}^{N-m} \pi_m(I^m(a_p; a_{p+1}, \ldots, a_{p+m}; a_{p+m+1}))
\]
\[ \otimes I^m(a_0; a_1, \ldots, a_p, a_{p+m+1}, \ldots, a_N; a_{N+1}). \]

As in [5, p.959], in the formula (4.1), we call the sequence of consecutive elements \( (a_p; a_{p+1}, \ldots, a_{p+m}; a_{p+m+1}) \) on the left a *subsequence of length* \( m \) of the original sequence and \( (a_0; a_1, \ldots, a_p, a_{p+m+1}, \ldots, a_N; a_{N+1}) \) a *quotient sequence*. For the subsequence \( (a_p; a_{p+1}, \ldots, a_{p+m}; a_{p+m+1}) \), we call the number of 1’s in \( \{a_{p+1}, \ldots, a_{p+m}\} \) the *depth*.

4.2. **A computation of the Brown operator** \( D_m \). The Brown operator for motivic multiple zeta values was computed in several papers ([4, 5] are the first). To keep this paper self-contained, we will give the formula. Following [22], we define \( \delta^{(m_1, \ldots, m_r)}_{(n_1, \ldots, n_r)} \) as the Kronecker delta given by
\[
\delta^{(m_1, \ldots, m_r)}_{(n_1, \ldots, n_r)} = \begin{cases} 
1 & \text{if } m_i = n_i \text{ for all } i \in \{1, \ldots, r\} \\
0 & \text{otherwise}
\end{cases}
\]
and the integer $b_{n,n'}^m (n,n', m \in \mathbb{Z})$ by
\[
  b_{n,n'}^m = (-1)^n \binom{m-1}{n-1} + (-1)^{n'-m} \binom{m-1}{n'-1},
\]
where $\binom{m}{n} = 0$ for each $n < 0$. It is obvious that for any odd integer $m > 1$ one has $b_{n,n'}^m + b_{n',n}^m = 0$.

**Definition 4.2.** For $r > 1$ and $r$-tuples of positive integers $(m_1, \ldots, m_r)$ and $(n_1, \ldots, n_r)$, we define
\[
e^{(m_1,\ldots,m_r)}_{(n_1,\ldots,n_r)} = \delta_{(m_1,\ldots,m_r)}^{(n_1,\ldots,n_r)} + \sum_{i=1}^{r-1} \delta_{(m_1,\ldots,m_i-1,m_i+2,\ldots,m_r)}^{(n_1,\ldots,n_i-1,n_i+2,\ldots,n_r)} b_{n_i,n_{i+1}}^m \in \mathbb{Z},
\]
and let $e^{(m_1)}_{(n_1)} = \delta_{(n_1)}^{(m_1)}$.

Let us denote by $\xi_m$ an image of $\zeta^m(m)$ in the space $L$ and by $\mathcal{D}_r H$ the $\mathbb{Q}$-vector space spanned by all motivic multiple zeta values of depth $\leq r$:
\[
\mathcal{D}_r H = \langle \zeta^m(n_1, \ldots, n_s) \mid n_1, \ldots, n_s \geq 1, 0 \leq s \leq r \rangle_{\mathbb{Q}}.
\]
We now compute the coefficient of $\xi_m \otimes \zeta^m(m_2, \ldots, m_r)$ in the formula $D_m(\zeta^m(n_1, \ldots, n_r))$.

**Proposition 4.3.** For any integers $n_1, \ldots, n_r \geq 1$ with $N = n_1 + \cdots + n_r$ and odd $m > 1$, the element
\[
D_m(\zeta^m(n_1, \ldots, n_r)) - \sum_{m_1 + \cdots + m_r = N, m_{1,\ldots,m_r} \geq 1} \delta_{(m_1,\ldots,m_r)}^{(n_1,\ldots,n_r)} e^{(m_1,\ldots,m_r)}_{(n_1,\ldots,n_r)} \xi_m \otimes \zeta^m(m_2, \ldots, m_r)
\]
lies in $L_m \otimes \mathcal{D}_{r-2} H_{N-m}$, where $\mathcal{D}_r H_N = \mathcal{D}_r H \cap H_N$.

**Proof.** Recall the formula (4.1). We apply $D_m$, with odd $m \geq 3$, to the element
\[
I^m(0; 1,0,\ldots,0,1,0,\ldots,0,1,0,\ldots,0,1,0; 0,1)_{n_1-1} \overbrace{0,0,\ldots,0}^{n_2-1} \overbrace{1,0,\ldots,0}^{n_r-1}
\]
Every subsequence of depth $\geq 2$ gives rise to a quotient sequence with $r - 2$ or less 1’s, so it lies in $L_m \otimes \mathcal{D}_{r-2} H_{N-m}$. We now consider the case when the subsequence is of depth 1. By the relations (3.7) and (3.9), every subsequence of depth 1 and length $m$ is one of the following two forms:

(a) $\overbrace{0,0,\ldots,0}^{n_1-1} 1,0,\ldots,0,0,1,0,\ldots,0,1,0; 0; 1)$,

(b) $\overbrace{0,0,\ldots,0}^{n_1-1} 1,0,\ldots,0,0,1,0,\ldots,0,0; 0)$. 

where \( i + j + 1 = m \) with \( i, j \geq 0 \). By (3.8), the case (b) is in turn computed from the case (a). For the case (a), using (3.6) and (3.9) repeatedly, one gets

\[
I^m(0; 0, \ldots, 0, 1, 0, \ldots, 0; 1) = \sum_{r+s=i+j \atop r, s \geq 0} (-1)^{r-j} \binom{r}{j} I^m(0; 1, 0, \ldots, 0; 1) I^m(0; 0, \ldots, 0; 1) = (-1)^i \binom{i+j}{j} \zeta^m(i+j+1).
\]

See also [5, Section 2.4]. Thus, every subsequence of depth 1 and length \( m \) produces an element in \( \mathbb{Q}\zeta_m \otimes \mathfrak{D}_{r-1}H_{N-m} \) (the depth on the right is of exactly \( r-1 \)). Summing these up, one obtains

\[
\sum_{m_1 + \cdots + m_r = N \atop m_1, \ldots, m_r \geq 1} \delta(m) e^{\binom{m_1, \ldots, m_r}{n_1, \ldots, n_r}} \xi_{m_1} \otimes \zeta^m(m_2, \ldots, m_r),
\]

which completes the proof. \( \Box \)

As special cases of Proposition 4.3, we have the following corollary, which we use later.

**Corollary 4.4.** (i) For integers \( N, n_1, n_2 \geq 1 \) with \( N = n_1 + n_2 \) and an odd integer \( m \) with \( N > m > 1 \), we have

\[
D_m(\zeta^m(n_1, n_2)) = e^{\binom{m,N-m}{n_1,n_2}} \xi_m \otimes \zeta^m(N-m).
\]

(ii) For integers \( N, n_1, n_2, n_3 \geq 1 \) with \( N = n_1 + n_2 + n_3 \) and an odd integer \( m \) with \( N > m > 1 \), we have

\[
D_m(\zeta^m(n_1, n_2, n_3)) = \sum_{k_1+k_2+k_3 = N \atop k_1, k_2, k_3 \geq 1} \delta(k) e^{\binom{k_1,k_2,k_3}{n_1,n_2,n_3}} \xi_{k_1} \otimes \zeta^m(k_2, k_3)
\]

\[+ a_m(n_1, n_2, n_3) \xi_m \otimes \zeta^m(N-m),\]

with some \( a_m(n_1, n_2, n_3) \in \mathbb{Q} \).

**Proof.** Since \( \mathfrak{D}_0H = \mathbb{Q} \), Corollary 4.4 (i) is immediate from Proposition 4.3. We now prove (ii). In this case, every subsequence has at most depth 2. By the parity result for double zeta values (see [28, Proposition 7]), we have

\[
\pi_m\left(I^k(0; 0, \ldots, 0, 1, 0, \ldots, 0; 1, 0, \ldots, 0; 1)\right) \in \mathbb{Q}\zeta_m.
\]

Thus, when the subsequence is of depth 2, it lies in \( \mathbb{Q}\zeta_m \otimes \zeta^m(N-m) \). This completes the proof. \( \Box \)
4.3. **Key lemma given by Brown.** We now define the infinitesimal version of the coaction \( \Delta^\bullet \) (see [5, Eq. (2.25)]). Set \( L := U_{>0}/(U_{>0})^2 \), which is a graded vector space \( L = \bigoplus_{m > 0} L_m \). Let \( \pi'_{m} : U_{>0} \to L_m \) be the projection. For each odd \( m > 1 \), let us define \( D_m^\bullet \) by the composition map

\[
D_m^\bullet : U \xrightarrow{\Delta^\bullet - 1 \otimes \text{id}} U_{>0} \otimes U \xrightarrow{\pi'_{m} \otimes \text{id}} L_m \otimes U.
\]

Note that using (3.11), one can easily compute \( D_m^\bullet \). By Theorem 3.1, the following diagram commutes:

\[
\begin{array}{ccc}
\mathcal{H} & \xrightarrow{D_m} & L_m \otimes \mathcal{H} \\
\downarrow \phi & & \downarrow \phi \otimes \phi,
\end{array}
\]

where \( \phi \) is the isomorphism

\[
\phi : L \to L
\]

induced by \( \phi \), which sends \( \xi_m \) to \( f_m := \pi'_m(f_m) \).

**Lemma 4.5.** ([5, Lemma 2.4]) We have

\[
\ker \sum_{1 < m < N \atop m \text{ odd}} D_m^\bullet |_{U_{>0}} = \mathbb{Q} f_N.
\]

4.4. **An explicit formula for \( \phi(\zeta^m(n_1, n_2)) \).** We now give an explicit formula for \( \phi(\zeta^m(n_1, n_2)) \).

**Proposition 4.6.** For any integer \( N, n_1, n_2 \geq 1 \) with \( N = n_1 + n_2 \), the image of \( \zeta^m(n_1, n_2) \) under the isomorphism \( \phi \) can be written in the form

\[
\phi(\zeta^m(n_1, n_2)) = \sum_{m_1 + m_2 = N \atop m_1 \geq 3 \text{ odd} \atop m_2 \geq 2} e^{m_1, m_2}_{n_1, n_2} f_{m_1} f_{m_2} + \tau(n_1, n_2) f_N
\]

with some \( \tau(n_1, n_2) \in \mathbb{Q} \).

**Proof.** From (4.2) and Corollary 4.4 (i), we have

\[
\sum_{1 < m < N \atop m \text{ odd}} D_m^\bullet \circ \phi(\zeta^m(n_1, n_2)) = \sum_{1 < m < N \atop m \text{ odd}} (\phi \otimes \phi) \circ D_m(\zeta^m(n_1, n_2))
\]

\[
= \sum_{1 < m < N \atop m \text{ odd}} e^{m, N-m}_{n_1, n_2} \overline{f}_m \otimes \overline{f}_{N-m},
\]

where we set \( f_1 = 0 \). On the other hand, the identity

\[
\sum_{1 < m < N \atop m \text{ odd}} D_m^\bullet \left( \sum_{m_1 + m_2 = N \atop m_1 \geq 3 \text{ odd} \atop m_2 \geq 2} e^{m_1, m_2}_{n_1, n_2} f_{m_1} f_{m_2} \right) = \sum_{m_1 + m_2 = N \atop m_1 \geq 3 \text{ odd} \atop m_2 \geq 2} e^{m_1, m_2}_{n_1, n_2} \overline{f}_m \otimes \overline{f}_{m_2}
\]
holds. Thus, one gets
\[ \phi(\zeta^m(n_1, n_2)) - \sum_{\substack{m_1+m_2=N \atop m_1 \geq 3; \text{odd}}} e^{(m_1, m_2)} f_{m_1} f_{m_2} \in \ker \sum_{1 < m < N \atop m: \text{odd}} D_m^*, \]
from which by Lemma 4.5 the assertion follows. \( \square \)

Let us illustrate an example. For \( N \) even, from \( e^{(m_1, m_2)} = \delta^{(m_1, m_2)} + b_{m_1, n_2} \) we have
\[ \phi(\zeta^m(1, N - 1)) + \sum_{\substack{m_1+m_2=N \atop m_1, m_2 \geq 3; \text{odd}}} f_{m_1} f_{m_2} \in \mathbb{Q} f_N. \]

With \( D_m \), we can not determine coefficients \( \tau(n_1, n_2) \) of \( f_N \) in the formula of Proposition 4.6. We use the rational solution to the double shuffle equation (see (4.4) below) to obtain \( \tau(n_1, n_2) \). Let
\[ (4.3) \quad \beta_k = -\frac{B_k}{2 \cdot k!}, \]
where \( B_k \) is the \( k \)-th Bernoulli number.

**Theorem 4.7.** Let \( N, n_1, n_2 \) be positive integers with \( N = n_1 + n_2 \geq 3 \). When \( N \) is even, we have
\[ \tau(n_1, n_2) = -\frac{1}{12} \left( 5 + (-1)^{n_1} \binom{N-1}{n_1} - (-1)^{n_1} \binom{N-1}{n_1-1} \right) \]
\[ + \frac{\beta_{n_1} \beta_{n_2}}{3 \beta_N} + \frac{(-1)^{n_1}}{3 \beta_N} \sum_{r=2}^{N} \binom{r-1}{n_2-1} \beta_r \beta_{N-r}. \]

When \( N \) is odd, we have
\[ \tau(n_1, n_2) = \frac{(-1)^{n_1+1}}{2} \left( (-1)^{n_1} + \binom{N-1}{r-1} + \binom{N-1}{s-1} \right). \]

**Proof.** In the case when \( N \) is even, we use the double shuffle relation satisfied by motivic double zeta values:
\[ \zeta^m(n_1) \zeta^m(n_2) = \zeta^m(n_1, n_2) + \zeta^m(n_2, n_1) + \zeta^m(N) \]
\[ = \sum_{m_1+m_2=N} \left( \binom{m_2-1}{n_1-1} + \binom{m_2-1}{n_2-1} \right) \zeta^m(m_1, m_2). \]

Applying the map \( \phi \) to the above equations and taking the coefficient of \( f_N \), one can deduce equations of \( \tau(r, s) \), which is called the double shuffle equation of depth 2:
\[ \frac{\beta_{n_1} \beta_{n_2}}{\beta_N} = \tau(n_1, n_2) + \tau(n_2, n_1) + 1 \]
\[ = \sum_{m_1+m_2=N} \left( \binom{m_2-1}{n_1-1} + \binom{m_2-1}{n_2-1} \right) \tau(m_1, m_2). \]
A solution to (4.3) is found in [11] Supplement to Proposition 5. More precisely, \( \tau(n_1, n_2) \) is obtained by the coefficient of \( x_1^{n_2-1} x_2^{n_1-1} \) in

\[
\frac{1}{3\beta_N} G_N(x_1, x_2) ((T^{-1} + 1) - \frac{1}{12} \frac{x_1^{N-1} - x_2^{N-1}}{x_1 - x_2}) (5 - 3U + U\varepsilon),
\]

where the matrices \( T, U, \varepsilon \) are defined in (3.1) and \( G_N(x_1, x_2) \) is defined by

\[
(4.5) \quad G_N(x_1, x_2) = \sum_{n_1 + n_2 = N, n_1, n_2 \geq 1} \beta_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1}.
\]

This is called the Bernoulli realization of the formal double zeta space in [11], Section 6] (with a small typo their \( Z_e \) corresponds to \( \tau(r, s) \) for \( r + s \) even).

In the case when \( N \) is odd, the result is obtained in the similar manner by the parity theorem given by Zagier [28, Proposition 7].

For example, one has

\[
\phi(\zeta^m(1, 4)) = 2f_5 - f_3f_2, \quad \phi(\zeta^m(2, 4)) = -\frac{4}{3} f_6 + 2f_3f_3, \quad \phi(\zeta^m(4, 2)) = \frac{25}{12} f_6 - 2f_3f_3.
\]

**Remark 4.8.** The isomorphism \( \phi \) is not unique, depending on the choice of \( \tau \). In [6, Section 7.3], Brown obtains another solution to (4.3), but our choice of \( \tau \) is easier for proving Theorem 2.2.

### 4.5. An explicit formula for \( \phi(\zeta^m(n_1, n_2, n_3)) \)

We now give an explicit formula for \( \phi(\zeta^m(n_1, n_2, n_3)) \). Our formula involves the following integers.

**Definition 4.9.** Let \( N, m_1, m_2, m_3, n_1, n_2, n_3 \) be positive integers such that \( N = m_1 + m_2 + m_3 = n_1 + n_2 + n_3, \) \( m_1, m_2 \geq 3 \) odd and \( m_3 \geq 2 \). We define the integer \( c(m_1, m_2, m_3) \) by

\[
c(m_1, m_2, m_3) = \sum_{k_1 + k_2 + k_3 = N} \delta_{k_1} e(m_2, m_3) e(k_1, k_2, k_3),
\]

where \( e(m_2, m_3) \) and \( e(k_1, k_2, k_3) \) are defined in Definition 4.2.

**Proposition 4.10.** Let \( N, n_1, n_2, n_3 \) positive integers with \( N = n_1 + n_2 + n_3 \). Then, we have

\[
\phi(\zeta^m(n_1, n_2, n_3)) - \sum_{m_1 + m_2 + m_3 = N, m_1, m_2 \geq 3 \text{ odd}} c(m_1, m_2, m_3) f_{m_1} f_{m_2} f_{m_3} \in U_N, 2
\]

where \( U_{N, 2} \) is the \( \mathbb{Q} \)-vector space spanned by \( f_{2n+1} f_{N-2n-1} \) \((1 \leq n < (N-1)/2) \) and \( f_N \).

**Proof.** By (4.2) and Corollary 4.4(ii), one computes

\[
D^*_{m_1} \circ \phi(\zeta^m(n_1, n_2, n_3)) = (\bar{\phi} \otimes \phi) \circ D_m(\zeta^m(n_1, n_2, n_3))
\]
$= \sum_{k_1+k_2+k_3=N \atop k_1,k_2,k_3 \geq 1} e^{(k_1,k_2,k_3)} \pi'_m(f_{k_1}) \otimes \phi(\zeta^m(k_2,k_3))$

$= \sum_{k_1+k_2+k_3=N \atop k_1,k_2,k_3 \geq 1} e^{(k_1,k_2,k_3)} \pi'_m(f_{k_1}) \otimes \phi(\zeta^m(k_2,k_3))$

$+ a_m(n_1,n_2,n_3) f_m \otimes f_{N-m}$,

and hence, by Proposition 4.6 and Definition 4.9, one obtains

$$\sum_{1 < m < N \atop m \text{ odd}} D_m^* \circ \phi(\zeta^m(n_1,n_2,n_3))$$

$$= \sum_{m_1+m_2+m_3=N \atop m_1,m_2 \geq 3; \text{odd} \atop m_3 \geq 2} c^{(m_1,m_2,m_3)} \pi'_m(f_{m_1}) \otimes f_{m_2} f_{m_3}$$

$$+ \sum_{1 < m < N \atop m \text{ odd}} a_m f_m \otimes f_{N-m}$$

with some $a_m \in \mathbb{Q}$. Note that

$$\sum_{1 < m < N \atop m \text{ odd}} D_m^* \left( \sum_{m_1+m_2+m_3=N \atop m_1,m_2 \geq 3; \text{odd} \atop m_3 \geq 2} c^{(m_1,m_2,m_3)} f_{m_1} f_{m_2} f_{m_3} \right)$$

$$= \sum_{m_1+m_2+m_3=N \atop m_1,m_2 \geq 3; \text{odd} \atop m_3 \geq 2} c^{(m_1,m_2,m_3)} \pi'_m(f_{m_1}) \otimes f_{m_2} f_{m_3}.$$

Hence

$$\phi(\zeta^m(n_1,n_2,n_3)) - \sum_{m_1+m_2+m_3=N \atop m_1,m_2 \geq 3; \text{odd} \atop m_3 \geq 2} c^{(m_1,m_2,m_3)} f_{m_1} f_{m_2} f_{m_3}$$

$$- \sum_{1 < m < N \atop m \text{ odd}} a_m f_m f_{N-m} \in \ker \sum_{1 < m < N \atop m \text{ odd}} D_m^*,$$

which completes the proof. \[\square\]

**Remark 4.11.** The above formula, together with explicit coefficients $a_m$ in the above proof, can also be computed by using explicit formulas for the Goncharov coproduct (see [1], Eq. (3.10) and Example 3.3]). Furthermore, the coefficient of $f_N$ in $\phi(\zeta^m(n_1,n_2,n_3))$ can be computed for $N$ odd by the parity theorem [21], Eq. (1.12)] and for $N$ even by the rational associator in depth 3 [8, Theorem 7.1]. We do not develop more explicit formula for $\phi(\zeta^m(n_1,n_2,n_3))$, since the formula is quite complicated and has no use in this paper.
5. Proof of Theorem 2.2

In this subsection, we first prepare some notations and then prove Theorem 2.2.
Throughout this subsection, we assume \( n \) is even \( \geq 4 \).

Now consider the square matrix
\[
E_N = \begin{pmatrix}
\tau(1, N - 1) + \frac{1}{2} e^{(3N-3)}_{N-1} & \cdots & e^{(3N-3)}_{N-1} \\
\tau(3, N - 3) + \frac{1}{2} e^{(3N-3)}_{3N-3} & \cdots & e^{(3N-3)}_{3N-3} \\
\vdots & \ddots & \vdots \\
\tau(N - 3, 3) + \frac{1}{2} e^{(3N-3)}_{N-3,3} & \cdots & e^{(3N-3)}_{N-3,3}
\end{pmatrix},
\]
which satisfies
\[
\begin{pmatrix}
\phi(\zeta^{m}_{1}(1, N - 1)) \\
\phi(\zeta^{m}_{2}(3, N - 3)) \\
\vdots \\
\phi(\zeta^{m}_{N}(N - 3, 3))
\end{pmatrix} = E_N \begin{pmatrix}
f_N \\
f_{3N-3} \\
\vdots \\
f_{N-3,N-3}
\end{pmatrix},
\]
where we set \( \zeta^{m}_{n_1,n_2}(n_1, n_2) = \zeta^{m}_{n_1,n_2}(n_1, n_2) + \frac{1}{2} \zeta^{m}_{n_1+n_2}. \) Since the size of the matrix \( E_N \) is \( N/2 - 1 \), if \( \text{rank} E_N < N/2 - 1 \), then there are linear relations among \( \zeta^{m}_{n_1,n_2}'s. \)

More precisely, we have the following lemma.

Lemma 5.1. The relation
\[
\sum_{\substack{n_1+n_2=N \\
n_1 \geq 1 \text{ odd} \\
n_2 \geq 3 \text{ odd}}} a_{n_1,n_2} \zeta^{m}_{n_1,n_2} = 0
\]
holds if and only if the row vector \( (a_{n_1,n_2}) \) is a left annihilator of the matrix \( E_N \).

Proof. This lemma follows from the fact that \( \phi \) is injective and the elements \( f_{\text{odd}}, f_{\text{odd}} \)'s and \( f_N \) are linearly independent over \( \mathbb{Q} \). \( \square \)

We now prove Theorem 2.2. In the proof, we do not hesitate to extend formally the algebras \( \mathcal{U} \) and \( \mathcal{H} \) over \( \mathbb{Q} \) to over \( \mathbb{C} \).

Proof of Theorem 2.2. Let \( a_{n_1,n_2} \) be the number defined in Theorem 2.2. Let \( P_{f}^{\text{ev},0}(x_1, x_2) = P_{f}^{\text{ev}}(x_1, x_2) - L_{f}^{*}(1)(x_1^{N-2} - x_2^{N-2}) \) and set
\[
P_{f}^{\text{ev},0}(x_1 + x_2, x_1) = \sum_{n_1+n_2=N} \binom{N-2}{n_1-1} q_{n_1,n_2} x_1^{n_1-1} x_2^{n_2-1}. 
\]
Since
\[
P_{f}^{\text{ev}}(x_1 + x_2, x_1) = P_{f}^{\text{ev},0}(x_1 + x_2, x_1) + L_{f}^{*}(1)(x_1 + x_2)^{N-2} - L_{f}^{*}(1)x_1^{N-2}, 
\]
it holds that \( a_{n_1,n_2} = q_{n_1,n_2} + L_f^*(1) \) unless \( n_2 = 1 \) (note \( q_{1,N-1} = 0 \)). With this, let us look at

\[
\sum_{n_1+n_2=N \atop n_1 \geq 1 \text{ odd}} a_{n_1,n_2} \zeta^m(n_1,n_2) = \sum_{n_1+n_2=N \atop n_1, n_2 \geq 3 \text{ odd}} q_{n_1,n_2} \zeta^m(n_1,n_2)
\]

\[+ L_f^*(1) \sum_{n_1+n_2=N \atop n_1 \geq 1 \text{ odd}} \zeta^m(n_1,n_2) + \frac{\zeta^m(N)}{2} \sum_{n_1+n_2=N \atop n_1 \geq 1 \text{ odd}} a_{n_1,n_2}. \tag{5.1} \]

Since \( P_{f}^{ev,0}(x_1,x_2) \in W_N^\infty \otimes \mathbb{C} \), it follows from [11, Theorem 3] and the restricted sum formula (2.2) (see below) that the first and the second term in the right hand-side of (5.1) lies in \( \mathbb{C} \zeta^m(N) \). Thus it suffices to check that the coefficient of \( f_N \) in the image of the left hand-side of (5.1) under the map \( \phi \) is 0. Namely, we prove

\[
\sum_{n_1+n_2=N \atop n_1 \geq 1 \text{ odd}} a_{n_1,n_2} \left( \tau(n_1,n_2) + \frac{1}{2} \right) = 0. \tag{5.2} \]

To prove this, we first recall the result of Kohnen and Zagier [16, Theorem 9]. Using the notation in Section 3.1, we define the paring \( \langle \cdot, \cdot \rangle : V_N^C \times V_N^C \to \mathbb{C} \) by

\[
\left\langle \sum_{n_1+n_2=N} a_{n_1,n_2} x_1^{n_1-1} x_2^{n_2-1}, \sum_{n_1+n_2=N} b_{n_1,n_2} x_1^{n_1-1} x_2^{n_2-1} \right\rangle \]

\[= \sum_{n_1+n_2=N} (-1)^{n_2} \binom{N-2}{n_1-1}^{-1} a_{n_1,n_2} b_{n_2,n_1}, \]

which is non-degenerate, symmetric. Moreover, the paring \( \langle \cdot, \cdot \rangle \) is \( \Gamma \)-invariant, i.e. for \( f, g \in V_N^\infty \) and \( \gamma \in \Gamma \) we have \( \langle f \big| \gamma, g \big| \gamma \rangle = \langle f, g \rangle \). For \( N = n_1 + n_2 \), let

\[
\lambda(n_1,n_2) = -\frac{\beta_N}{12} \left( 1 + (-1)^{n_1} \binom{N-1}{n_1-1} - (-1)^{n_1} \binom{N-1}{n_1} \right)
\]

\[= -\frac{(-1)^{n_1}}{3} \sum_{r=2}^{N} \binom{r-1}{n_2-1} \beta_r \beta_{N-r}. \]

Note that it holds that

\[
\lambda(n_1,n_2) = -\beta_N \tau(n_1,n_2) - \frac{\beta_N}{2} + \frac{\beta_{n_1} \beta_{n_2}}{3},
\]

where \( \tau(n_1,n_2) \) is given in Theorem 4.4. With this notation, Kohnen and Zagier showed that for any \( f \in S_N \) we have

\[
\left\langle P_f^{ev}(x_1,x_2), \sum_{n_1+n_2=N} \lambda(n_1,n_2) x_1^{n_1-1} x_2^{n_2-1} \right\rangle = 0. \tag{5.3} \]
Let us turn to the proof of (5.2). Consider
\[
\Phi_N(x_1, x_2) = \sum_{n_1 + n_2 = N} (\tau(n_1, n_2) + \frac{1}{2})x_1^{n_1-1}x_2^{n_2-1}
\]
\[
= -\frac{1}{\beta_N} \sum_{n_1 + n_2 = N} \lambda(n_1, n_2)x_1^{n_1-1}x_2^{n_2-1} + \frac{1}{3\beta_N}G_N(x_1, x_2),
\]
where \(G_N(x_1, x_2)\) is defined in (4.5). With the matrices defined in (3.1), we see that the identity (5.2) is equivalent to
\[
\langle P_f^{ev}(x_1, x_2)\big| T, \Phi_N(x_1, x_2)\big| (1 + \delta) \rangle = 0.
\]
Let \(W\) be the left hand-side:
\[
W = \langle P_f^{ev}(x_1, x_2)\big| T, \Phi_N(x_1, x_2)\big| (1 + \delta) \rangle
\]
\[
= \langle P_f^{ev}(x_1, x_2)\big| T\varepsilon, \Phi_N(x_1, x_2)\big| (1 + \delta)\varepsilon \rangle.
\]
By the period relation \(P_f^{ev}(x_1, x_2)\big| (1 - T + T\varepsilon) = 0\), one can compute
\[
2W = \langle P_f^{ev}(x_1, x_2)\big| T, \Phi_N(x_1, x_2)\big| (1 + \delta) \rangle
\]
\[
+ \langle P_f^{ev}(x_1, x_2)\big| T\varepsilon, \Phi_N(x_1, x_2)\big| (1 + \delta)\varepsilon \rangle
\]
\[
= \langle P_f^{ev}(x_1, x_2)\big| T, \Phi_N(x_1, x_2)\big| (1 + \delta) \rangle
\]
\[
+ \langle P_f^{ev}(x_1, x_2)\big| (T - 1), \Phi_N(x_1, x_2)\big| (1 + \delta)\varepsilon \rangle
\]
\[
= \langle P_f^{ev}(x_1, x_2)\big| T, \Phi_N(x_1, x_2)\big| (1 + \varepsilon)(1 + \delta) \rangle
\]
\[
- \langle P_f^{ev}(x_1, x_2), \Phi_N(x_1, x_2)\big| (1 + \delta)\varepsilon \rangle.
\]
Since \(\tau(n_1, n_2) + \tau(n_2, n_1) + 1 = \beta_n\beta_n/\beta_N\), one has
\[
\Phi_N(x_1, x_2)\big| (1 + \varepsilon)(1 + \delta) = \frac{1}{\beta_N}G_N(x_1, x_2),
\]
and hence, \(\Phi_N(x_1, x_2)\big| (1 + \varepsilon)(1 + \delta) = 0\). By \(P_f^{ev}(x_1, x_2)\big| (1 + \varepsilon) = 0\), we have
\[
2W = \langle P_f^{ev}(x_1, x_2), \Phi_N(x_1, x_2)\big| (1 + \delta) \rangle = 2\langle P_f^{ev}(x_1, x_2), \Phi_N(x_1, x_2)\rangle.
\]
By (5.3) and \(\langle P_f^{ev}(x_1, x_2), G_N(x_1, x_2)\rangle = 0\), we obtain
\[
\langle P_f^{ev}(x_1, x_2), \Phi_N(x_1, x_2)\rangle = 0,
\]
and hence \(W = 0\), from which the identity (5.2) follows. We complete the proof. \(\square\)

Remark 5.2. Corollary 2.3 is obtained by substituting Theorem 2.2 and the restricted sum formula (2.2) into the equation (5.1). Theorems 2.4 and 2.5 may be immediate from [17 Theorems 1 and 2] and [18 Lemma 5.1]; the details are left to the reader.
6. Linear relations among almost totally odd motivic triple zeta values

6.1. Almost totally odd motivic multiple zeta values. Denote by $\mathcal{D}$ the depth filtration (see [6, Section 4]), which is an increasing filtration on $\mathcal{H}$:

$$\mathcal{D}_0 \mathcal{H} = \mathcal{Q} \subset \mathcal{D}_1 \mathcal{H} \subset \cdots \subset \mathcal{D}_r \mathcal{H} \subset \cdots \subset \mathcal{H}.$$ 

We note that the space $\mathcal{H}$ has the structure of a filtered algebra with respect to the depth filtration $\mathcal{D}$, i.e.

$$\mathcal{D}_r \mathcal{H} \cdot \mathcal{D}_s \mathcal{H} \subset \mathcal{D}_{r+s} \mathcal{H}$$

holds for any $r, s \geq 0$.

Consider the following graded $\mathbb{Q}$-algebra:

$$\text{gr}^{\mathcal{D}} \mathcal{H} := \bigoplus_{r \geq 1} \mathcal{D}_r \mathcal{H} / \mathcal{D}_{r-1} \mathcal{H}.$$ 

We denote by

$$\zeta^{\mathcal{D}}_m(n_1, \ldots, n_r)$$

an image of $\zeta_m(n_1, \ldots, n_r)$ in the bigraded $\mathbb{Q}$-algebra $\text{gr}^{\mathcal{D}} \mathcal{H}$, called the depth-graded motivic multiple zeta value. Note that by definition $\zeta^{\mathcal{D}}_m(2)$ is non-zero. Now we define the $j$-th almost totally odd motivic multiple zeta value.

**Definition 6.1.** For an integer $r \geq j \geq 1$, the depth-graded motivic multiple zeta value $\zeta^{\mathcal{D}}_m(n_1, \ldots, n_r)$ is called a $j$-th almost totally odd motivic multiple zeta value if $n_j \geq 2$ is even and other $n_i$’s are odd and greater than 1.

The reminder of this subsection is devoted to illustrating some expectation for the almost totally odd motivic multiple zeta values. As a prototype, we have in mind an analogues story for the study of totally odd motivic multiple zeta values developed by Brown [6, Section 10]. They are elements $\zeta_m(2n_1 + 1, 2n_2 + 1, \ldots, 2n_r + 1)$’s ($n_i \geq 1$) in the space $\text{gr}^{\mathcal{D}} \mathcal{A}$, with $\mathcal{A} := \mathcal{H} / \zeta_m(2) \mathcal{H}$. In [6, Conjecture 4], Brown recast the Broadhurst-Kreimer conjecture [3] as a statement of the homology of the depth-graded motivic Lie algebra $\mathfrak{d}$ (see [3, Section 2.5] and [6, Section 4]). It is believed that the $\mathbb{Q}$-algebra generated by totally odd motivic multiple zeta values is isomorphic to the graded dual of the universal enveloping algebra of the Lie subalgebra $\mathfrak{g}^{\text{odd}}$ of $\mathfrak{d}$ generated by canonical generators $\sigma^{(1)}_{2i+1}$ in depth 1. The generators $\sigma^{(1)}_{2i+1}$ are also believed to be subject only to the quadratic relations obtained from restricted even period polynomials (the Ihara-Takao relation). These lead to the uneven part of the Broadhurst-Kreimer conjecture [6, Conjecture 5] stating that the generating series of the dimension of the $\mathbb{Q}$-vector space spanned by all totally odd multiple zeta values of weight $N$ and depth $r$ is given by

$$\frac{1}{1 - \mathcal{D}(x)y + \mathcal{S}(x)y^2}.$$
Now consider the \( \mathbb{Q} \)-vector space \( \mathcal{H}_r^{al} \) spanned by \( \zeta_S^n(2n_1)\zeta_S^n(2n_2 + 1, \ldots, 2n_r + 1) \) \( (n_i \geq 1) \) of weight \( N \) and depth \( r \) for positive integers \( N > r > 1 \). We let \( \mathcal{H}_{N,1}^{al} = \mathbb{Q} \zeta^{\mathfrak{o}}_S(N) \) if \( N \) is even and \( \mathcal{H}_{N,1}^{al} = \{0\} \) if \( N \) is odd. According to the Conjecture 2.10 and (6.1) (note that by Theorem 6.4 below we have\[ j \]
which does not depend on \( j \).

Indeed, the equality of the coefficients of \( y^r \) in (6.1) holds for \( r = 1, 2, 3 \) (the case \( r = 3 \) is due to Goncharov [12]).

Denote by \( \mathcal{H}_{N,r}^{al,(j)} \) the \( \mathbb{Q} \)-vector space spanned by all \( j \)-th almost totally odd motivic multiple zeta values of weight \( N \) and depth \( r \). By the parity theorem we have \( \mathcal{H}_{N,r}^{al,(j)} \subset \mathcal{H}_{N,r}^{al} \) for \( r = 1, 2, 3 \) and \( 1 \leq j \leq r \), which is not known for \( r \geq 4 \). Moreover, it follows from [28, Theorem 2] (see also [19]) that the equality \( \mathcal{H}_{N,2}^{al,(1)} = \mathcal{H}_{N,2}^{al} \) holds. According to Conjecture 2.10 and (6.1) (note that by Theorem 6.4 below we have dim \( \mathcal{H}_{N,3}^{al,(2)} = \text{rank} C^{(2)}_N \)), it is expected that the equality \( \mathcal{H}_{N,3}^{al,(2)} = \mathcal{H}_{N,3}^{al} \) holds. In general, we are expecting the following conjecture.

**Conjecture 6.2.** For \( N > r \geq 3 \), we have \( \mathcal{H}_{N,r}^{al,(r-1)} = \mathcal{H}_{N,r}^{al} \).

**6.2. Matrices \( C^{(j)}_N \).** Hereafter, we will restrict our attention to the \( j \)-th almost totally odd motivic triple zeta value. We define the matrices \( C^{(j)}_N \) mentioned in the introduction and clarify the meaning of the right (resp. left) annihilator of them.

Let
\[
\mathbb{I}^{(j)}_N
\]
be the set of \( j \)-th almost totally odd indices of weight \( N \) and depth 3. They are \( \mathbb{I}^{(1)}_N = \mathbb{I}_N(\mathfrak{o}\mathfrak{o}\mathfrak{o}), \mathbb{I}^{(2)}_N = \mathbb{I}_N(\mathfrak{o}\mathfrak{e}\mathfrak{o}), \mathbb{I}^{(3)}_N = \mathbb{I}_N(\mathfrak{o}\mathfrak{e}\mathfrak{e}) \) (see [25]). Set
\[
d_N = |\mathbb{I}^{(j)}_N|,
\]
which does not depend on \( j \). Note that \( \sum_{N>0} d_N x^N = E(x)O(x)^2 \).

**Definition 6.3.** For each integer \( N > 0 \) and \( j \in \{1, 2, 3\} \), the \( d_N \times d_N \) matrix \( C_N^{(j)} \) is defined by
\[
C_N^{(j)} = (c_{n\mathfrak{m}}^{(j)})_{\mathfrak{m} \in \mathbb{I}^{(j)}_N, \mathfrak{n} \in \mathbb{I}^{(j)}_N},
\]
whose rows and columns are indexed by \( \mathfrak{m} \) and \( \mathfrak{n} \) in the sets \( \mathbb{I}^{(3)}_N \) and \( \mathbb{I}^{(j)}_N \), respectively, where the integers \( c_{n\mathfrak{m}}^{(j)} \) are defined in Definition 4.9.

In the next subsection, we shall discuss the right annihilators of the matrix \( C_N^{(j)} \). Before doing this, we introduce vector spaces \( \text{Vect}_N^{(j)} \) \( (j = 1, 2, 3) \) and specify the meaning of the right (and left) annihilators of the matrix \( C_N^{(j)} \).
For \( j \in \{1, 2, 3\} \), we denote by \( \text{Vect}_N^{(j)} \) the \( d_N \)-dimensional vector space over \( \mathbb{Q} \) of row vectors \( (a_n)_{n \in I_N^{(j)}} \) indexed by \( j \)-th almost totally odd indices \( n \in I_N^{(j)} \) with rational coefficients:

\[
\text{Vect}_N^{(j)} = \{ (a_n)_{n \in I_N^{(j)}} \mid a_n \in \mathbb{Q} \}.
\]

The matrix \( C_N^{(j)} \) induces a linear map from \( \text{Vect}_N^{(3)} \) to \( \text{Vect}_N^{(j)} \):

\[
C_N^{(j)} : \text{Vect}_N^{(3)} \rightarrow \text{Vect}_N^{(j)}
\]

so that, for a row vector \( v = (a_n)_{n \in I_N^{(3)}} \in \text{Vect}_N^{(3)} \), we have

\[
C_N^{(j)}(v) = \left( \sum_{m \in I_N^{(3)}} a_m c(m)^{n} \right)_{n \in I_N^{(j)}},
\]

where we regard \( C_N^{(j)} \) as an empty matrix (i.e. \( \text{rank} C_N^{(j)} = 0 \)) when \( d_N = 0 \). It is clear that a row vector \( v = (a_n)_{n \in I_N^{(3)}} \in \text{Vect}_N^{(3)} \) satisfies \( C_N^{(j)}(v) = 0 \) if and only if

\[
\sum_{m \in I_N^{(3)}} a_m c(m)^{n} = 0
\]

for all \( n \in I_N^{(j)} \). Hereafter, we denote by \( \text{ker} C_N^{(j)} \) the subspace of \( \text{Vect}_N^{(3)} \) consisting of left annihilators of the matrix \( C_N^{(j)} \).

Since each matrix \( C_N^{(j)} \) is square, the equality

\[
\dim_{\mathbb{Q}} \ker C_N^{(j)} = \dim_{\mathbb{Q}} \ker C_N^{(j)}
\]

holds, where the space \( \ker C_N^{(j)} \), which is a subspace of \( \text{Vect}_N^{(j)} \), describes all right annihilators of the matrix \( C_N^{(j)} \). We note that the linear map \( \tau C_N^{(j)} : \text{Vect}_N^{(j)} \rightarrow \text{Vect}_N^{(3)} \) is given for \( v = (a_n)_{n \in I_N^{(3)}} \) by

\[
\tau C_N^{(j)}(v) = \left( \sum_{n \in I_N^{(j)}} a_n c(m)^{n} \right)_{m \in I_N^{(3)}}.
\]

6.3. Right annihilators of the matrix \( C_N^{(j)} \). In this subsection, we prove that the dimension of the \( \mathbb{Q} \)-vector space spanned by all \( j \)-th almost totally odd motivic triple zeta values of weight \( N \) equals the rank of the matrix \( C_N^{(j)} \), namely, \( \dim \mathcal{H}_{N,3}^{\text{al}(j)} = \text{rank} C_N^{(j)} \). This is an immediate consequence of the following theorem.

**Theorem 6.4.** Let \( N \) be a positive even integer. For \( j \in \{1, 2, 3\} \), the \( \mathbb{Q} \)-linear relation of the form

\[
\sum_{n \in I_N^{(j)}} a_n c_m^{n}(\mathbf{1}) = 0
\]
holds if and only if the row vector \((a_n)_{n \in I_N^{(j)}}\) lies in \(\ker C_N^{(j)}\).

**Proof.** Let \((a_n)_{n \in I_N^{(j)}}\) be an element in \(\ker C_N^{(j)}\). Set

\[
\xi = \sum_{n \in I_N^{(j)}} a_n \zeta_n^m(n).
\]

From Proposition 1.10 one has \(\phi(\xi) \in \mathcal{U}_{N,2}\). On the other hand, by the parity theorem (see [22], for example) \(\xi\) can be written in terms of double zeta values \(\zeta(\text{odd, odd})\) and single zeta values

\[
(6.3) \quad \xi = \sum_{(m_1, n_2, m_3) \in \mathbb{I}_N^{(3)}} b_{m_1, n_2, m_3} \zeta_m(n_1, n_2) \zeta_m(n_3) + \gamma
\]

with some \(b_{m_1, n_2, m_3} \in \mathbb{Q}\) and \(\gamma \in \mathcal{D}_2 \mathcal{H}_N\). Since by Proposition 1.6 the element

\[
(6.4) \quad \phi \left( \sum_{n_1 + n_2 = N_n - n_3 \atop n_1, n_2 \geq 3 \atop n_1, n_2 \text{ odd}} b_{n_1, n_2, n_3} \zeta_m(n_1, n_2) \zeta_m(n_3) \right)
\]

lies in the \(\mathbb{Q}\)-vector space spanned by \(f_{odd} f_{odd} f_{n_3}'s\) and \(f_N\), (6.4) is a rational multiple of \(f_N\), and hence, \(\xi \in \mathcal{D}_2 \mathcal{H}_N\).

Conversely, suppose that we have

\[
\xi = \sum_{n \in I_N^{(j)}} a_n \zeta_n^m(n) \in \mathcal{D}_2 \mathcal{H}_N.
\]

It is easily seen that the identity \((\text{id} \otimes \mathcal{D}_{m_2}) \circ \mathcal{D}_{m_1}(\xi) = 0\) holds for all \((m_1, m_2, m_3) \in \mathbb{I}_N^{(3)}\) because \(\xi \in \mathcal{D}_2 \mathcal{H}_N\). With this, the statement that \((a_n)_{n \in I_N^{(3)}} \in \ker C_N^{(j)}\) can be checked by using Corollary 4.4 and then Definition 4.9.

Let us illustrate a few examples of linear relations obtained from Theorem 6.4.

**Example 6.5.** For the matrix \(C_N^{(3)}\), the first non-trivial linear relation is obtained from the matrix

\[
C_{12}^{(3)} = \begin{pmatrix}
\begin{pmatrix}
7.3.2 & 7.3.2 & 7.3.2 & 7.3.2 & 7.3.2 & \cdots & 7.3.2
\end{pmatrix} \\
\begin{pmatrix}
5.5.2 & 5.5.2 & 5.5.2 & 5.5.2 & 5.5.2 & \cdots & 5.5.2
\end{pmatrix} \\
\begin{pmatrix}
3.7.2 & 3.7.2 & 3.7.2 & 3.7.2 & 3.7.2 & \cdots & 3.7.2
\end{pmatrix} \\
\begin{pmatrix}
7.3.2 & 7.3.2 & 7.3.2 & 7.3.2 & 7.3.2 & \cdots & 7.3.2
\end{pmatrix} \\
\begin{pmatrix}
5.5.2 & 5.5.2 & 5.5.2 & 5.5.2 & 5.5.2 & \cdots & 5.5.2
\end{pmatrix} \\
\begin{pmatrix}
3.7.2 & 3.7.2 & 3.7.2 & 3.7.2 & 3.7.2 & \cdots & 3.7.2
\end{pmatrix} \\
\begin{pmatrix}
7.3.2 & 7.3.2 & 7.3.2 & 7.3.2 & 7.3.2 & \cdots & 7.3.2
\end{pmatrix} \\
\begin{pmatrix}
5.5.2 & 5.5.2 & 5.5.2 & 5.5.2 & 5.5.2 & \cdots & 5.5.2
\end{pmatrix} \\
\end{pmatrix}
\end{pmatrix}
\]
For $N > 0$ even, consider

$$C^{(\text{eee})}_{N} = \left( c^{(m_1,m_2,m_3)}_{n_1,n_2,n_3} \right)_{(m_1,m_2,m_3) \in I_N^{(3)}, (n_1,n_2,n_3) \in I_N^{(\text{eee})}}$$

Remark 6.6. The technique we have used can also be applied to the case $\zeta_B^m(\text{even, even, even})$. For $N > 0$ even, consider

$$C^{(\text{eee})}_{N} = \left( c^{(m_1,m_2,m_3)}_{n_1,n_2,n_3} \right)_{(m_1,m_2,m_3) \in I_N^{(3)}, (n_1,n_2,n_3) \in I_N^{(\text{eee})}}.$$
where $\mathbb{I}_N(\text{eee})$ is the set of all indices $(n_1, n_2, n_3)$ of weight $N$ with $n_i$ even (see also (2.5)). For this, one can show that

$$\dim_\mathbb{Q}(\mathcal{C}_N^m(n_1, n_2, n_3) | (n_1, n_2, n_3) \in \mathbb{I}_N(\text{eee}))_\mathbb{Q} = \text{rank } C_N^{(\text{eee})}.$$  

Our numerical experiment suggests that

$$\sum_{N>0} \text{rank } C_N^{(\text{eee})} x^N = E(x)^3 - O(x)^2 - E(x)S(x) = E(x)O(x)^2 - E(x)S(x).$$

This dimension conjecture implies that the $\mathbb{Q}$-vector space $\mathcal{H}_{N,3}^\text{reg}$ spanned by elements $\zeta_\mathbb{Q}^3(n_1)\zeta_\mathbb{Q}^3(n_2, n_3)$ ($(n_1, n_2, n_3) \in \mathbb{I}_N(\text{eee})$) is generated by $\zeta_\mathbb{Q}^3(n_1, n_2, n_3)$ ($(n_1, n_2, n_3) \in \mathbb{I}_N(\text{eee})$), which was also pointed out by M. Hirose and N. Sato.

7. Proof of Theorem 2.7

7.1. A key lemma. In this subsection, we first prove certain identities of polynomials, and then give another expression of the integer $c(m_1, m_2, m_3)_{n_1, n_2, n_3}$.

For a Laurent polynomial $f(x_1, x_2, x_3) \in \mathbb{Q}[x_1^{\pm 1}, x_2^{\pm 1}, x_3^{\pm 1}]$, consider the following change of variables:

$$f(x_1, x_2, x_3)|\sigma_1 = f(x_2 - x_1, x_1, x_3) - f(x_2 - x_1, x_2, x_3),$$

$$f(x_1, x_2, x_3)|\sigma_2 = f(x_3 - x_2, x_1, x_2) - f(x_3 - x_2, x_1, x_3),$$

$$f(x_1, x_2, x_3)|\sigma_3 = f(x_1, x_2 - x_3, x_2) - f(x_1, x_2 - x_3, x_3),$$

$$f(x_1, x_2, x_3)|\sigma_4 = f(x_2 - x_1, x_3 - x_1, x_1) - f(x_2 - x_3, x_2, x_2),$$

$$f(x_1, x_2, x_3)|\sigma_5 = f(x_3 - x_2, x_3 - x_1, x_3) - f(x_2 - x_3, x_2 - x_1, x_2).$$

**Lemma 7.1.** For any Laurent polynomial $f(x_1, x_2, x_3) \in \mathbb{Q}[x_1^{\pm 1}, x_2^{\pm 1}, x_3^{\pm 1}]$ satisfying $f(\pm x_1, \pm x_2, x_3) = f(x_1, x_2, x_3)$, we have

$$f(1 + \sigma_3)|\sigma_3(1 + \sigma_1 + \sigma_2) = f(1 + \sigma_1)\sigma_1(1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5),$$

where $f(1 + \sigma_3)$ means $f + f|\sigma_3$.

**Proof.** The proof is straightforward. For instance, one can check

$$f(x_1, x_2, x_3)|\sigma_1|\sigma_2 = f(x_1 - x_3 + x_2, x_3 - x_2, x_2) - f(x_1 - x_3 + x_2, x_1, x_2)$$

$$- f(x_1 - x_3 + x_2, x_3 - x_2, x_3) + f(x_1 - x_3 + x_2, x_1, x_3).$$

Computing each term and then using the assumption that $f(\pm x_1, \pm x_2, x_3) = f(x_1, x_2, x_3)$ holds, we can verify the identity (7.2). □

By comparing the coefficients of both sides of the identity (7.2), we obtain another expression of the integer $c(m_1, m_2, m_3)_{n_1, n_2, n_3}$. 
For integers $m_1, m_2, m_3, n_1, n_2, n_3 \geq 1$, let us define an integer $h(m_1, m_2, m_3)$ by the formula
\[
 h(m_1, m_2, m_3) = \delta(m_1, m_2, m_3) + \delta(m_2, n_1, n_2, n_3) + \delta(m_1, n_3, n_2, n_3) \\
+ (-1)^{m_1+2+m_3}(m_2-1) \left( (-1)^{n_2} \left( \frac{m_1 - 1}{n_2 - 1} \right) - (-1)^{n_1} \left( \frac{m_1 - 1}{n_1 - 1} \right) \right) \\
+ (-1)^{n_1} \left( \frac{m_2 - 1}{n_1 - 1} \right) \left( (-1)^{n_2} \left( \frac{m_1 - 1}{n_2 - 1} \right) - (-1)^{n_3} \left( \frac{m_1 - 1}{n_3 - 1} \right) \right).
\]
(7.3)

Write $a = o \cup e$, meaning the set of all integers $> 1$.

**Corollary 7.2.** Let $N > 0$ be an even integer and $j \in \{1, 2, 3\}$. For any $(m_1, m_2, m_3) \in \mathbb{Z}_N^{(3)}$ and $(n_1, n_2, n_3) \in \mathbb{I}_N^{(j)}$, we have
\[
 c(m_1, m_2, m_3) = \sum_{(k_1, k_2, k_3) \in \mathbb{I}_N^{(aa)}} e(m_1, m_2, m_3) \delta(k_3) h(k_1, k_2, k_3).
\]

**Proof.** This is an exercise and left to the reader. \hfill \Box

### 7.2. Proof of Theorem 2.7

In this subsection, we give a proof of Theorem 2.7.

**Proof of Theorem 2.7** By Corollary 7.2, the matrix $C_{(j)}^{(j)}$ is written as follows:
\[
 C_{N}^{(j)} = \left(e(m_1, m_2, m_3) \delta(n_3)\right)_{(m_1, m_2, m_3) \in \mathbb{I}_N^{(3)}} \cdot \left(h(m_1, m_2, m_3)\right)_{m \in \mathbb{I}_N^{(aa)}}.
\]

The first term can be written in terms of a block matrix with blocks $C_{N-k}$ for $k = 2, 4, \ldots, N - 6$:
\[
 \left(e(m_1, m_2, m_3) \delta(n_3)\right)_{(m_1, m_2, m_3) \in \mathbb{I}_N^{(3)}} = \text{diag}(C_{N-2}, C_{N-4}, \ldots, C_6),
\]
where for $N > 0$ even, the matrix $C_N$ is defined by
\[
 C_N = \left(e(m_1, m_2, m_3)\right)_{m \in \mathbb{I}_N^{(aa)}},
\]
whose rows and columns are indexed by $m$ and $n$ in the sets $\mathbb{I}_N^{(oo)}$ and $\mathbb{I}_N^{(aa)}$, respectively. Then, Theorem 2.7 follows from the fact that the map
\[
 W_N^Y \rightarrow \ker C_N
\]

\[
 \sum_{(n_1, n_2) \in \mathbb{I}_N^{(oo)}} a_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1} \rightarrow (a_n, n)_{(n_1, n_2) \in \mathbb{I}_N^{(oo)}}
\]
is an isomorphism as $Q$-vector spaces, which is a consequence of [22 Proposition 3.2] (see also [22 Proposition 3.4]). We complete the proof. \hfill \Box

**Remark 7.3.** As we described in the introduction, there have to be more elements in $\ker C_N^{(1)}$ corresponding to the $x^N$-term in
\[
 \frac{1}{x^2} E(x) S(x) - E(x) S(x) = S(x),
\]
which is nothing but the cusp forms of weight $N$. For this, the first author observed a remarkable connection with the “derivative” of odd period polynomials removing the first and last terms (which should be called the restricted odd period polynomial). For example, the row vector $(35, -42, 15, 0, 0)$ is a basis of $\ker C^{(1)}_N$, and these coefficients are obtained from the derivative of the odd period polynomial \(2.4\) ignoring the terms $4x_1^0 x_2 + 4x_1 x_2^0$. In general, for $p(x_1, x_2) \in W^\text{od}_N$, let $a_{n_1,n_2,n_3}$ be the coefficient of $x_1^{n_1-1} x_2^{n_2-1} x_3^{n_3-1}$ in
\[
\frac{x_3}{x_2} \frac{dp}{dx_1}(x_1, x_2).
\]
Then, the row vector $(a_n)_{n \in I_N^{(3)}}$ seemingly lies in $\ker C^{(1)}_N$. This phenomena was verified by Mathematica up to $N = 40$.

8. Proofs of Theorems 2.8 and 2.9

8.1. Definition. In this subsection, we define matrices $B_N^{(3)}$ and $E_N^{(3)}$.

Definition 8.1. The $d_N \times d_N$ matrices $B_N^{(3)}$ and $E_N^{(3)}$ (recall $d_N = |I_N^{(3)}|$) are defined by
\[
B_N^{(3)} = \left( \delta^{(m_1)}_{n_1} e^{(m_2,m_3)}_{n_2,n_3} \right)_{(m_1,m_2,m_3) \in I_N^{(3)}};
\]
\[
E_N^{(3)} = \left( \epsilon^{(m_1,m_2,m_3)}_{n_1,n_2,n_3} \right)_{(m_1,m_2,m_3) \in I_N^{(3)}};
\]
whose rows and columns are indexed by $(m_1, m_2, m_3)$ and $(n_1, n_2, n_3)$ in the set $I_N^{(3)}$, respectively.

Proposition 8.2. For any $N > 0$ even, we have $C_N^{(3)} = B_N^{(3)} \cdot E_N^{(3)}$.

Proof. By Definition 4.9 for any $(m_1, m_2, m_3), (n_1, n_2, n_3) \in I_N^{(3)}$, the identity
\[
e^{(m_1,m_2,m_3)}_{n_1,n_2,n_3} = \sum_{(k_1,k_2,k_3) \in I_N^{(3)}} \delta^{(m_1)}_{k_1} e^{(m_2,m_3)}_{k_2,k_3} e^{(k_1,k_2,k_3)}_{m_1,m_2,m_3}
\]
holds, because $\delta^{(m_1)}_{k_1} e^{(m_2,m_3)}_{k_2,k_3} e^{(k_1,k_2,k_3)}_{n_1,n_2,n_3} = 0$ holds for $(k_1, k_2, k_3) \not\in I_N^{(3)}$. Thus, we complete the proof.

8.2. Proof of Theorem 2.8. We give a proof of Theorem 2.8.

Proof of Theorem 2.8. By definition, the matrix $B_N^{(3)}$ can be written in terms of a block diagonal matrix with blocks $B_{N-k}$ for $k = 3, 5, \ldots, N - 5$:
\[
B_N^{(3)} = \text{diag}(B_{N-3}, B_{N-5}, \ldots, B_3),
\]
where the matrix $B_N$ is defined by
\begin{equation}
B_N = \left( e^{\left( \frac{m_1 m_2}{n_1 n_2} \right)} \right)_{(m_1, m_2) \in \mathbb{I}_{N}^{(\text{oe})}}.
\end{equation}

The matrix $B_N$ was studied by Zagier [28, Section 6], and his result induces Theorem 2.8. Since his matrix is slightly different from the matrix $B_N$, we recall the result of [28, Section 6] with a brief sketch of the proof.

It is easily seen that the assertion that a row vector $(a_{n_1, n_2})_{(n_1, n_2) \in \mathbb{I}_{N}^{(\text{oe})}}$ lies in $\ker B_N$ is equivalent to the statement that the polynomial $q(x_1, x_2) = \sum_{(n_1, n_2) \in \mathbb{I}_{N}^{(\text{oe})}} a_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1}$ satisfies
\[ q(x_1, x_2) - q(x_2 - x_1, x_2) + q(x_2 - x_1, x_1) = (\text{odd polynomial in } x_1). \]

With this, one can easily check that the map
\[
W_{N-1}^{\text{od}} \mapsto \ker B_N
\]
\[ p(x_1, x_2) = \sum_{(n_1, n_2) \in \mathbb{I}_{N-1}^{(\text{oe})}} a_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1} \mapsto (a_{n_1-1, n_2})_{(n_1, n_2) \in \mathbb{I}_{N}^{(\text{oe})}}, \]
where the image is the coefficient vector of $x_1 p(x_1, x_2)$, and the map
\[
W_{N+1}^{\text{ev}} \mapsto \ker B_N
\]
\[ p(x_1, x_2) = \sum_{(n_1, n_2) \in \mathbb{I}_{N+1}^{(\text{oe})}} a_{n_1, n_2} x_1^{n_1-1} x_2^{n_2-1} \mapsto (n_2 a_{n_2+1, n_1})_{(n_1, n_2) \in \mathbb{I}_{N}^{(\text{oe})}}, \]
where the image is the coefficient vector of $\frac{d p}{d x_1}(x_2, x_1)$, are well-defined. By definition, the injectivity of each of these maps separately is obvious. The injectivity of the combined map is also obvious since the images have incompatible symmetry properties. □

Remark 8.3. It is expected that
\[
\sum_{N \geq 0} \dim \ker B_N^{(3)} x_N \geq (x + \frac{1}{x}) \mathcal{O}(x) S(x),
\]
which has been checked by Mathematica up to $N = 40$. For this, Theorem 2.8 gives the best lower bound of $\dim \ker B_N^{(3)}$.

8.3. **Proof of Theorem 2.9** In order to describe the linear map from $\hat{\mathbf{P}}_N^{(3)} \cap \ker B_N^{(3)}$ in Theorem 2.9, we use the following notations. Consider an extended index set of $\mathbb{I}_N^{(3)}$ allowing the cases when $n_3 = 0$:
\[
\hat{\mathbb{I}}_N^{(3)} = \{ \mathbf{n} = (n_1, n_2, n_3) \in \mathbb{Z}_{\geq 0}^3 \mid n_1, n_2 \in \text{o, } n_3 \geq 0 \text{ : even} \}.
\]

Its associated vector space is denoted by $\hat{\text{\text{Vect}}}_N^{(3)}$:
\[
\hat{\text{\text{Vect}}}_N^{(3)} = \{ (a_{\mathbf{n}})_{\mathbf{n} \in \hat{\mathbb{I}}_N^{(3)}} \mid a_{\mathbf{n}} \in \mathbb{Q} \}. 
\]
Our target space $\text{Im} B^{(3)}_N \cap \ker E^{(3)}_N$, which is a subspace of $\text{Vect}^{(3)}_N$, can be embedded into the space of $\widehat{\text{Vect}}^{(3)}_N$ via the embedding $i_0 : \text{Vect}^{(3)}_N \rightarrow \widehat{\text{Vect}}^{(3)}_N$ given by

$$i_0 : \text{Vect}^{(3)}_N \rightarrow \widehat{\text{Vect}}^{(3)}_N$$

$$(a_n)_{n \in \mathbb{N}}^{(3)} \mapsto (a_n)_{n \in \mathbb{N}}^{(3)}.$$

where we simply put $a_{2n+1,N-2n-1,0} = 0$ for all $1 \leq n \leq N/2 - 2$.

Let $\widehat{\Phi}^*_N$ be the $|\hat{I}(N)|$-dimensional $\mathbb{Q}$-vector space spanned by the set $\{x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1} \mid (n_1, n_2, n_3) \in \hat{I}(N)\}$, which is isomorphic to the space $\widehat{\text{Vect}}^{(3)}_N$. The isomorphism is denoted by $\rho(=\rho^{(N)});$:

$$\rho : \widehat{\Phi}^*_N \rightarrow \widehat{\text{Vect}}^{(3)}_N$$

$$x_1^{m_1-1}x_2^{m_2-1}x_3^{m_3-1} \mapsto (\delta(m_1,m_2,m_3))_{(n_1,n_2,n_3) \in \hat{I}(N)}.$$  

We note that the space $\hat{\Phi}^{ev}_N$ is a subspace of $\widehat{\Phi}^*_N$, and hence the space $\rho(\hat{\Phi}^{ev}_N)$ is a subspace of $\widehat{\text{Vect}}^{(3)}_N$. With this notation, the precise statement of Theorem 2.9 is given as follows.

**Theorem 8.4.** Let $N > 0$ be an even integer. Define the square matrix $L_N$ by

$$L_N = (e^{\binom{m}{n}} - \delta^{\binom{m}{n}})_{n \in \hat{I}(N)},$$

which is viewed as a linear map on $\widehat{\text{Vect}}^{(3)}_N$. Then, the map

$$L_N : \rho(\hat{\Phi}^{ev}_N) \rightarrow i_0(\text{Im} B^{(3)}_N \cap \ker E^{(3)}_N)$$

is well-defined as a $\mathbb{Q}$-linear map.

**Proof.** The proof is done by showing the following claims:

(1) $L_N(\rho(\hat{\Phi}^{ev}_N)) \subset i_0(\ker E^{(3)}_N)$,

(2) $L_N(\rho(\hat{\Phi}^{ev}_N)) \subset i_0(\text{Im} B^{(3)}_N)$,

from which, by $i_0(\text{Im} B^{(3)}_N \cap \ker E^{(3)}_N) = i_0(\text{Im} B^{(3)}_N) \cap i_0(\ker E^{(3)}_N)$, Theorem 8.4 follows.

(1) Define the square matrix $\hat{E}^{(3)}_N$ by

$$\hat{E}^{(3)}_N = (e^{\binom{m}{n}})_{n \in \hat{I}(N)},$$

We first prove $L_N(\rho(\hat{\Phi}^{ev}_N)) \subset \hat{E}^{(3)}_N$, and then $L_N(\rho(\hat{\Phi}^{ev}_N)) \subset i_0(\ker E^{(3)}_N)$.

For $p(x_1, x_2, x_3) \in \hat{\Phi}^{ev}_N$, by the relation satisfied by even period polynomial we have

$$p(x_1, x_2, x_3)(1 + \sigma_1) = 0,$$

where $\sigma_1$ is defined in (7.1). We also have

$$p(x_1, x_2, x_3) + \rho(x_2, x_1, x_3) = 0,$$
which is equivalent to the antisymmetry property of the coefficients of even period polynomials. Using these two relations, one can check that the following identity holds:

\[(\rho|\sigma_1 + \sigma_2)(1 + \sigma_1 + \sigma_2) = 0,\]

which is a special case of \[\text{(3.31)}\]. Computing the coefficients, one easily sees that for each \((n_1, n_2, n_3) \in \mathbb{I}^{(3)}_N\)

the coefficient of \(x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}\) in \((\rho|\sigma_1 + \sigma_2)(1 + \sigma_1 + \sigma_2)\)

\[= (n_1, n_2, n_3)\text{-th entry of the row vector } \rho(p) \cdot L_N \cdot \hat{E}^{(3)}_N,\]

so by \[\text{(8.4)}\] we have \(L_N(\rho(\hat{P}^{(3)}_N)) \subset \ker \hat{E}^{(3)}_N\).

Let us turn to the proof of the inclusion \(L_N(\rho(\hat{P}^{(3)}_N)) \subset i_0(\ker B^{(3)}_N)\). For \(p \in \hat{P}^{(3)}_N\), we write \(\rho(p) = (a_n)_{n \in \mathbb{I}^{(3)}_N}\) and \(L_N(\rho(p)) = (c_n)_{n \in \mathbb{I}^{(3)}_N}\). Since \(e(m_1,m_2,m_3) = 0\) whenever \(m_3 > 0\) and \(n_2 = 0\), for \(n_1, n_2 \geq 3\) odd with \(n_1 + n_2 = N\) we see that

\[
c_{n_1,n_2,0} = \sum_{m_1+m_2=N \atop m_1,m_2 \geq 3: \text{odd}} a_{m_1,m_2,0} \left( e^{(m_1,m_2,0)} - \delta^{(m_1,m_2)}_{(m_1,n_2,0)} \right) \\
= \sum_{m_1+m_2=N \atop m_1,m_2 \geq 3: \text{odd}} a_{m_1,m_2,0} \left( \delta^{(m_1,m_2)}_{(n_1,n_2,0)} - \delta^{(m_2,m_1)}_{(n_1,n_2,0)} \right) \\
= \sum_{m_1+m_2=N \atop m_1,m_2 \geq 3: \text{odd}} a_{m_1,m_2,0} \left( \delta^{(m_2,m_1)}_{(n_1,n_2,0)} + \delta^{(m_1,m_2)}_{(n_1,n_2,0)} \right) = 0,
\]

where for the third equality we have used \[\text{(8.3)}\] and for the last equality we have used the relation \[\text{(8.2)}\]. Since we have shown \(L_N(\rho(p)) \in \ker \hat{E}^{(3)}_N\), for any \(n \in \mathbb{I}^{(3)}_N\) it follows

\[0 = \sum_{m \in \mathbb{I}^{(3)}_N} c_ne^{(m)}_n.\]

Since \(c_{n_1,n_2,0} = 0\), we find that for any \(n \in \mathbb{I}^{(3)}_N\) the relation

\[0 = \sum_{m \in \mathbb{I}^{(3)}_N} c_ne^{(m)}_n\]

holds. This implies that the row vector \((c_n)_{n \in \mathbb{I}^{(3)}_N}\) lies in \(\ker E^{(3)}_N\), so the claim 1 is done.

(Claim 2). Let us prove the inclusion \(L_N(\rho(\hat{P}^{(3)}_N)) \subset i_0(\ker B^{(3)}_N)\). Define the square matrix \(\hat{B}^{(3)}_N\) by

\[\hat{B}^{(3)}_N = \delta^{(m_1)}_{(n_1)} e^{(m_2,m_3)}_{(n_2,n_3)} \text{ for } (m_1,m_2,m_3) \in \mathbb{I}^{(3)}_N.\]

We first prove \(L_N(\rho(\hat{P}^{(3)}_N)) = \hat{B}^{(3)}_N(\rho(\hat{P}^{(3)}_N))\), and then \(\hat{B}^{(3)}_N(\rho(\hat{P}^{(3)}_N)) \subset i_0(\Im B^{(3)}_N).\)
Lemma 8.5. For each odd integer $N \geq 3$, there exists an element $(a_n)_{n \in \mathbb{N}(\infty)} \in \ker \widehat{B}_N$ such that $a_{N,0} \neq 0$.

Proof. Since $\widehat{B}_3 = (a^{3,0}_n) = (0)$, we have $\ker \widehat{B}_3 = \mathbb{Q}$. For the case $N \geq 5$ odd, such element in the statement is obtained from the extended period polynomial corresponding to the Eisenstein series, which was developed in [25]. For $N = 2$ even, let

$$
\widehat{G}_N(x_1, x_2) := 4 \sum_{n_1+n_2=N \atop n_1,n_2 \geq 0} \beta_{n_1} \beta_{n_2} x_1^{k_1-1} x_2^{k_2-1},
$$

where $\beta_N$ is defined in [13] (note that the Laurent polynomial $\widehat{G}_N(x_1, x_2)$ corresponds to [25 Eq. (11)]). It follows that $\widehat{G}_N(x_1, x_2) = \widehat{G}_N(x_2, x_1)$. For $N \geq 5$ odd, we set $p(x_1, x_2) = x_1 \widehat{G}_{N-1}(x_1, x_2)$ and define rational numbers $a_{n_1,n_2}$’s by

$$
(8.5) \quad p(x_1, x_2) - p(0, x_2) = \sum_{(n_1,n_2) \in \mathbb{N}(\infty)} a_{n_1,n_2} x_1^{n_1-1} x_2^{n_2-1}.
$$

Since $a_{N,0} \neq 0$, the proof is done by showing that the row vector $(a_n)_{n \in \mathbb{N}(\infty)}$ lies in $\ker \widehat{B}_N$.

It can be shown that the assertion that a row vector $(a_n)_{n \in \mathbb{N}(\infty)}$ lies in $\ker \widehat{B}_N$ is equivalent to the statement that the polynomial $q(x_1, x_2) = \sum_{(n_1,n_2) \in \mathbb{N}(\infty)} a_{n_1,n_2} x_1^{n_1-1} x_2^{n_2-1}$ satisfies

$$
q(x_1, x_2) - q(x_2 - x_1, x_2) + q(x_2 - x_1, x_1) = (\text{odd polynomial in } x_1).
$$
Now let us denote by \( q(x_1, x_2) \) the left-hand side of (8.5). By [25 Proposition in p.453] and [11 Lemma in p.14], it follows that
\[
\hat{G}_N(x_1, x_2) - \hat{G}_N(x_1 + x_2, x_2) - \hat{G}_N(x_1 + x_2, x_1) = 0,
\]
and hence
\[
p(x_1, x_2) = x_1(\hat{G}_{N-1}(x_1 + x_2, x_2) + \hat{G}_{N-1}(x_1 + x_2, x_1)),
p(x_2, x_1) = x_2\hat{G}_{N-1}(x_2, x_1) = x_2\hat{G}_{N-1}(x_1, x_2)
= x_2(\hat{G}_{N-1}(x_1 + x_2, 2x_2) + \hat{G}_{N-1}(x_1 + x_2, x_1)).
\]
Combining the above equations, one has
\[
p(x_1, x_2) = -p(x_2, x_1) + p(x_1 + x_2, x_2) + p(x_1 + x_2, x_1).
\]
Then, one obtains
\[
q(x_1, x_2) - q(x_2 - x_1, x_2) + q(x_2 - x_1, x_1)
= -p(x_2, x_1) + p(x_2 + x_1, x_1) + p(x_2 - x_1, x_1) - p(0, x_1).
\]
By definition, it is easily seen that the right-hand is an odd polynomial in \( x_1 \), so the proof is concluded.

Let us turn to the proof of the inclusion \( \hat{B}_N^{(3)}(\rho(\hat{P}_N^{(3)})) \subset i_0(\text{Im } B_N^{(3)}) \). It suffices to show that for any \( v \in \rho(\hat{P}_N^{(3)}) \), there exists \( v' \in \text{Vect}_N^{(3)} \) such that
\[
\hat{B}_N^{(3)}(v) = i_0(B_N^{(3)}(v')).
\]
We note that the matrix \( \hat{B}_N^{(3)} \) can be written in terms of a block diagonal matrix with blocks \( \hat{B}_{N-k} \) for \( k = 3, 5, \ldots, N - 3 \):
\[
\hat{B}_N^{(3)} = \text{diag}(\hat{B}_{N-3}, \hat{B}_{N-5}, \ldots, \hat{B}_3).
\]
By Lemma [8.5], for each \( (m_1, m_2) \in I_N(\text{oo}) \), one can obtain a row vector \( v_{m_1,m_2} \in \ker \hat{B}_N^{(3)} \) whose \( (n_1, n_2, 0) \)-th entry is \( \delta_{m_1,m_2}^{(n_1,n_2)} \) for all \( (n_1, n_2, 0) \in I_N^{(3)}(3) \). Then, for any \( \rho(p) = (a_n)_{n \in I_N^{(3)}(3)} \in \rho(\hat{P}_N) \), the element
\[
\rho(p) = \sum_{(n_1,n_2) \in I_N(\text{oo})} a_{n_1,n_2,0} \cdot v_{n_1,n_2}
\]
lies in \( i_0(\text{Vect}_N^{(3)}) \). This shows that there is an element \( v' \in \text{Vect}_N^{(3)} \) satisfying \( \hat{B}_N^{(3)}(\rho(p)) = \hat{B}_N^{(3)}(i_0(v')) \). Since \( e_{m,N-m}^{(n,N,0)} = 0 \) whenever \( N - m > 0 \), it is easily seen that the equality \( \hat{B}_N^{(3)}(i_0(v')) = i_0(B_N^{(3)}(v')) \) holds. Hence \( \hat{B}_N^{(3)}(\rho(\hat{P}_N^{(3)})) \) belongs to \( i_0(\text{Im } B_N^{(3)}) \), so does \( L_N(\rho(\hat{P}_N^{(3)})) \).
Remark 8.6. We expect that the map $L_N$ in Theorem 8.4 is bijective, because our numerical experiments suggest

$$\text{Im} E_N^{(3)} \cap \ker E_N^{(3)} = \ker E_N^{(3)}$$

and

$$\sum_{N>0} \dim \ker E_N^{(3)} x^N = \frac{1}{x^2} E(x) S(x),$$

which have both been verified by using Mathematica up to $N = 40$.

9. The parity result for depth 3

A consequence of Corollary 7.2 and Theorem 8.4 one can give an explicit formula for the parity result for $c_{\overline{S}}(n_1, n_2, n_3)$ with $(n_1, n_2, n_3) \in \mathbb{I}_N^{(j)}$. A similar result is found [21, Eq. (1.12)] (but not known that his formula is lifted to motivic multiple zeta values), and his formula is different from the formula below due to linear relations among multiple zeta values.

**Theorem 9.1.** Let $N > 0$ be an even integer. For each $(n_1, n_2, n_3) \in \mathbb{I}_N^{(j)}$, we have

$$\zeta_{\overline{D}}^m(n_1, n_2, n_3) = \sum_{(k_1, k_2, k_3) \in I_N(aae)} h_{(n_1, n_2, n_3)}(k_1, k_2, k_3) \zeta_{\overline{D}}^m(k_1, k_2, k_3),$$

where $h_{(n_1, n_2, n_3)} \in \mathbb{Z}$ is defined in [13].

**Proof.** It suffices to show that for any $(n_1, n_2, n_3) \in \mathbb{I}_N^{(j)}$, we have

$$\zeta^m(n_1, n_2, n_3) = \sum_{(k_1, k_2, k_3) \in I_N(aae)} h_{(n_1, n_2, n_3)}(k_1, k_2, k_3) \zeta^m(k_1, k_2, k_3) \in \mathcal{D}_2 \mathcal{H}_N.$$

By the parity theorem, we know that there exist some rational numbers and $\gamma \in \mathcal{D}_2 \mathcal{H}_N$ such that

$$\zeta^m(n_1, n_2, n_3) = \sum_{(k_1, k_2, k_3) \in I_N(aae)} a_{(n_1, n_2, n_3)}(k_1, k_2, k_3) \zeta^m(k_1, k_2, k_3) + \gamma. \quad (9.1)$$

By Corollary 7.2 and Proposition 4.10 we have

$$\phi\left(\zeta^m(n_1, n_2, n_3) - \sum_{(k_1, k_2, k_3) \in I_N(aae)} h_{(n_1, n_2, n_3)}(k_1, k_2, k_3) \zeta^m(k_1, k_2, k_3) - \gamma\right) \in \mathcal{U}_{N, 2}.$$

By (9.1), the left-hand side of the above is reduced to

$$\phi\left(\sum_{(k_1, k_2, k_3) \in I_N(aae)} \left(a_{(n_1, n_2, n_3)}(k_1, k_2, k_3) - h_{(n_1, n_2, n_3)}(k_1, k_2, k_3)\right) \zeta^m(k_1, k_2, k_3)\right). \quad (9.2)$$

Since by Proposition 4.6 for $(n_1, n_2, n_3) \in I_N(aae)$ we have

$$\phi(\zeta^m(n_1, n_2) \zeta^m(n_3)) \in \langle f_{m_1} f_{m_2} f_{m_3} \mid (m_1, m_2, m_3) \in I_N^{(3)} \rangle \mathcal{Q} \oplus \mathbb{Q} f_N,$$
it turns out that the element (9.2) lies in $\mathbb{Q}_fN$, and hence
\[
\phi \left( \zeta^m(n_1, n_2, n_3) - \sum_{(k_1, k_2, k_3) \in I_N(\text{ane})} h(k_1, k_2, k_3) \zeta^m(k_1, k_2) \zeta^m(k_3) - \gamma \right) \in \mathbb{Q}_fN.
\]
This completes the proof. □

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