Double Shuffle Relations for Refined Symmetric Multiple Zeta Values

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Abstract. Symmetric multiple zeta values (SMZVs) are elements in the ring of all multiple zeta values modulo the ideal generated by $\zeta(2)$ introduced by Kaneko-Zagier as counterparts of finite multiple zeta values. It is known that symmetric multiple zeta values satisfy double shuffle relations and duality relations. In this paper, we construct certain lifts of SMZVs which live in the ring generated by all multiple zeta values and $2\pi i$ as certain iterated integrals on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ along a certain closed path. We call these lifted values refined symmetric multiple zeta values (RSMZVs). We show double shuffle relations and duality relations for RSMZVs. These relations are refinements of the double shuffle relations and the duality relations of SMZVs. Furthermore, we compare RSMZVs to other variants of lifts of SMZVs. Especially, we prove that RSMZVs coincide with Bachmann-Takeyama-Tasaka's ξ-values.

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1 Introduction

For an index $\mathbb{k} = (k_1, \ldots, k_d)$, the multiple zeta value $\zeta(\mathbb{k})$ is the real number defined by

$$\zeta(\mathbb{k}) = \sum_{0<m_1<\cdots<m_d} m_1^{-k_1} \cdots m_d^{-k_d}$$

where $k_1,\dots,k_{d-1}\in\mathbb{Z}_{\geq 1}$ and $k_d\in\mathbb{Z}_{\geq 2}$. Let $\mathcal{Z}$ be the $\mathbb{Q}$-subalgebra of $\mathbb{R}$ generated by 1 and all multiple zeta values. The symmetric multiple zeta value (SMZV) is the element of $\mathcal{Z}/\pi^2\mathcal{Z}$ defined by

$$\zeta^S(k_1,\dots,k_d) := \left(\sum_{i=0}^{d}(-1)^{k_{i+1}+\cdots+k_d}\zeta_{ш}(k_1,\dots,k_i)\zeta_{ш}(k_d,\dots,k_{i+1}) \mod \pi^2\mathcal{Z}\right)$$

for $k_1,\dots,k_d\in\mathbb{Z}_{\geq 1}$ where $\zeta_{ш}(\Bbbk)$ is the shuffle regularized multiple zeta value. SMZVs are introduced by Kaneko and Zagier as counterparts of finite multiple zeta values [8][9]. In this paper, we define *refined symmetric multiple zeta values* (RSMZV) $\zeta^{RS}(\Bbbk)\in\mathcal{Z}[2\pi i]=\mathcal{Z}\oplus 2\pi i\mathcal{Z}$ by considering iterated integrals along the non-trivial simple path from 0 to 0 on $\mathbb{P}^1(\mathbb{C})\setminus\{0,1,\infty\}$ (see Figure 2.3), and show the following properties:

- $\zeta^{RS}(\Bbbk)$ is a lift of $\zeta^S(\Bbbk)$ i.e., $\rho(\zeta^{RS}(\Bbbk))=\zeta^S(\Bbbk)$ where $\rho:\mathcal{Z}[2\pi i]\xrightarrow{\mathrm{Re}}\mathcal{Z}\to\mathcal{Z}/\pi^2\mathcal{Z}$ (Corollary 6).
- ζ^{RS} satisfies double shuffle relations, duality relations, and reversal formula (Theorems 8 and 10).
- ζ^{RS} coincides with Bachmann-Takeyama-Tasaka's ξ-value in [1, Definition 2.12] (see Remark 13).

The contents of this paper are as follows. In Section 2, we give a definition of RSMZVs and show some basic facts. In Section 3, we formulate the double shuffle relations, and prove the duality relation and the reversal formula. In Section 4, we consider other variants of SMZVs and compare them to RSMZVs, and give a proof of the double shuffle relations. In Section 5, we present some complementary results.

2 Iterated integral expression of refined symmetric multiple zeta values

2.1 Iterated integral symbols

Let us introduce some notions concerning (regularized) iterated integrals. Our basic references are [2] and [3, Section 2]. We define a *tangential base point* v_p as a pair of a point $p\in\mathbb{C}$ and a nonzero tangential vector $v\in T_p\mathbb{C}=\mathbb{C}$. We define a *path* from v_p to w_q on a subset $M\subset\mathbb{C}$ as a continuous piecewise smooth map $\gamma:[0,1]\to\mathbb{C}$ such that $\gamma(0)=p$, $\gamma'(0)=v$, $\gamma(1)=q$, $\gamma'(1)=-w$ and $\gamma(t)\in M$ for all $0<t<1$. We denote by $\pi_1(M,v_p,w_q)$ the set of homotopy classes of paths from v_p to w_q on M. For tangential base points x,y,z and a subset $M\subset\mathbb{C}$, the composition map

$$\pi_1(M,x,y)\times\pi_1(M,y,z)\to\pi_1(M,x,z)\quad;\quad(\gamma_1,\gamma_2)\mapsto\gamma_1\gamma_2$$

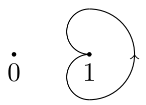

Figure 2.1: the path α

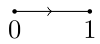

Figure 2.2: the path dch

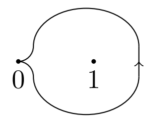

Figure 2.3: the path β

and the inverse map

$$\pi_1(M, x, y) \to \pi_1(M, y, x) \quad ; \quad \gamma \mapsto \gamma^{-1}$$

are naturally defined.

Definition 1. Fix complex numbers $a_1, \dots, a_n \in \mathbb{C}$ and tangential base points x, y. For $\Gamma \in \pi_1(\mathbb{C} \setminus \{a_1, \dots, a_n\}, x, y)$, we define $I_\Gamma(x; a_1, \dots, a_n; y) \in \mathbb{C}$ as follows. For a representative γ of Γ, define the function $F_\gamma : (0, \frac{1}{2}) \to \mathbb{C}$ by

$$F_\gamma(t) := \int_{t<t_1<\cdots<t_n<1-t} \prod_{j=1}^{n} \frac{d\gamma(t_j)}{\gamma(t_j) - a_j}.$$

Then there exist complex numbers $c_0, c_1, \dots, c_n \in \mathbb{C}$ such that

$$F_\gamma(t) = \sum_{k=0}^{n} c_k (\log t)^k + O(t \log^{n+1} t)$$

for $t \to 0$. It is known that $c_0, \dots, c_n$ do not depend on the choice of γ (see [2, Proposition 3.238]). We define $I_\Gamma(x; a_1, \dots, a_n; y) := c_0$. (In this notation, the information of tangential base points x, y is redundant, however, we do not omit them to conform to the standard notations).

If $p \neq a_1$ and $q \neq a_n$ then this is just a usual iterated integral i.e.,

$$I_{[\gamma]}(v_p; a_1, \dots, a_n; w_q) = \int_{0<t_1<\cdots<t_n<1} \prod_{j=1}^{n} \frac{d\gamma(t_j)}{\gamma(t_j) - a_j}.$$

2.2 Definition and explicit expression of refined symmetric multiple zeta values

We define two tangential basepoints $0'$ and $1'$ by

$$0' = 1_0, \ 1' = (-1)_1.$$

Put $M = \mathbb{C} \setminus \{0, 1\}$. Let dch $\in \pi_1(M, 0', 1')$ be (the homotopy class represented by) the straight line from $0'$ to $1'$, $\alpha \in \pi_1(M, 1', 1')$ the path from $1'$ to $1'$ which circles 1 one times counterclockwise, and $\beta = \mathrm{dch} \cdot \alpha \cdot \mathrm{dch}^{-1}$ the path from $0'$ to $0'$ which circles 1 one times counterclockwise (see Figure 2.1, 2.2 and 2.3).

Note that

$$\begin{aligned}(-1)^d\zeta_{\sqcup\!\sqcup}(k_1,\dots,k_d) &= I_{\mathrm{dch}}(0';1,\overbrace{0,\dots,0}^{k_1-1},\dots,1,\overbrace{0,\dots,0}^{k_d-1};1')\\ &= (-1)^{k_1+\cdots+k_d} I_{\mathrm{dch}^{-1}}(1';\overbrace{0,\dots,0}^{k_d-1},1,\dots,\overbrace{0,\dots,0}^{k_1-1},1;0')\end{aligned}$$

and

$$I_\alpha(1';a_1,\dots,a_n;1') = \begin{cases}\frac{(2\pi i)^n}{n!} & a_1=\cdots=a_n=1\\ 0 & \text{otherwise}\end{cases}$$

for $a_1,\dots,a_n\in\{0,1\}$ (see [2, Theorem 3.251 and Examples 3.259]).

Definition 2. For $d\geq 0$ and $k_1,\dots,k_d\in\mathbb{Z}_{\geq 1}$, we define the refined symmetric multiple zeta value $\zeta^{RS}(k_1,\dots,k_d)\in\mathbb{C}$ by

$$\zeta^{RS}(k_1,\dots,k_d) := \frac{(-1)^d}{2\pi i} I_\beta(0';1,\overbrace{0,\dots,0}^{k_1-1},\dots,1,\overbrace{0,\dots,0}^{k_d-1},1;0').$$

For example, $\zeta^{RS}(3,2) = \frac{1}{2\pi i}I(0';1,0,0,1,0,1;0')$ and $\zeta^{RS}(\emptyset) = \frac{1}{2\pi i}I_\beta(0';1;0')=1$.

Remark 3. In [7, Definition A.1.2 (i)], Jarossay defined the *exponential adjoint cyclotomic multiple zeta values* by

$$\begin{aligned}&\zeta^{\exp,\mathrm{Ad}}\big((n_i)_d;(\xi_i)_{d+1};l\big)\\ &\quad:= \sum_{\xi\in\mu_N(\mathbb{C})} \xi^{-1}(x\mapsto \xi x)_*(\Phi_{\mathrm{KZ}}^{-1}e^{2i\pi e_1}\Phi_{\mathrm{KZ}})[e_0^l e_{\xi_{d+1}} e_0^{n_d-1}e_{\xi_d}\dots e_0^{n_1-1}e_{\xi_1}].\end{aligned}$$

Here $N,n_1,\dots,n_d$ are positive integers, l is a nonnegative integer, $\mu_N(\mathbb{C})$ is the set of N-th roots of unity, $\xi_1,\dots,\xi_{d+1}$ are elements of $\mu_N(\mathbb{C})$, Φ_{KZ} is the noncommutative power series defined by

$$\Phi_{\mathrm{KZ}} := \sum_{k=0}^{\infty}\sum_{a_1,\dots,a_k\in\{0\}\cup\mu_N(\mathbb{C})} I_{\mathrm{dch}}(1';a_1,\dots,a_k;0')e_{a_1}\cdots e_{a_k},$$

and $(\Phi_{\mathrm{KZ}}^{-1}e^{2i\pi e_1}\Phi_{\mathrm{KZ}})[e_0^l e_{\xi_{d+1}} e_0^{n_d-1}e_{\xi_d}\dots e_0^{n_1-1}e_{\xi_1}]$ is the coefficient of $e_0^l e_{\xi_{d+1}} e_0^{n_d-1}e_{\xi_d}\dots e_0^{n_1-1}e_{\xi_1}$ in $\Phi_{\mathrm{KZ}}^{-1}e^{2i\pi e_1}\Phi_{\mathrm{KZ}}$. Let $N=1$ and $l=0$. The author could not find the definition of $(x\mapsto\xi x)_*$ in [7], but if we assume that $(x\mapsto\xi x)_*$ is the identity map for $\xi=1$, then $\zeta^{\exp,\mathrm{Ad}}\big((n_i)_d;(\xi_i)_{d+1};l\big)=\zeta^{\exp,\mathrm{Ad}}\big((n_i)_d;(1)_{d+1};0\big)$ is equal to

$$I_\beta(0';1,\overbrace{0,\dots,0}^{n_d-1},\dots,1,\overbrace{0,\dots,0}^{n_1-1},1;0') = (-1)^d 2\pi i\zeta^{RS}(n_d,\dots,n_1)$$

by the path composition formula.

There are several ways to express RSMZVs by multiple zeta values. We give one of such expressions obtained by a most naive way here (see Corollary 12 for other expressions).

Proposition 4. *We have*

$$\zeta^{RS}(k_1,\dots,k_d) = \sum_{\substack{0\le a\le b\le d \\ k_j=1 \text{ for all } a<j\le b}} \frac{(-2\pi i)^{b-a}}{(b-a+1)!}(-1)^{k_{b+1}+\cdots+k_d}\zeta_{ш}(k_1,\dots,k_a)\zeta_{ш}(k_d,\dots,k_{b+1}).$$

Proof. Let $n=k_1+\cdots+k_d+1$ and $(a_1,\dots,a_n):=(1,\overbrace{0,\dots,0}^{k_1-1},\dots,1,\overbrace{0,\dots,0}^{k_d-1},1)$. Then from the path composition formula, we have

$$\begin{aligned} I_\beta(0';a_1,\dots,a_n;0') &= \sum_{0\le l\le m\le n} I_{\mathrm{dch}}(0';a_1,\dots,a_l;1')I_\alpha(1';a_{l+1},\dots,a_m;1') \\ &\qquad \times I_{\mathrm{dch}^{-1}}(1';a_{m+1},\dots,a_n;0') \\ &= \sum_{\substack{0\le l\le m\le n \\ a_j=1 \text{ for all } l<j\le m}} \frac{(2\pi i)^{m-l}}{(m-l)!} I_{\mathrm{dch}}(0';a_1,\dots,a_l;1')I_{\mathrm{dch}^{-1}}(1';a_{m+1},\dots,a_n;0'). \end{aligned}$$

Here, again from the path composition formula, we have

$$\sum_{0\le l=m\le n} I_{\mathrm{dch}}(0';a_1,\dots,a_l;1')I_{\mathrm{dch}^{-1}}(1';a_{m+1},\dots,a_n;0') = I_{\mathrm{dch}\cdot\mathrm{dch}^{-1}}(0';a_1,\dots,a_n;0')=0.$$

Thus

$$
\begin{aligned}
&I_\beta(0';a_1,\dots,a_n;0')\\
&=\sum_{\substack{0\le l<m\le n\\ a_j=1 \text{ for all } l<j\le m}}\frac{(2\pi i)^{m-l}}{(m-l)!}I_{\mathrm{dch}}(0';a_1,\dots,a_l;1')I_{\mathrm{dch}^{-1}}(1';a_{m+1},\dots,a_n;0')\\
&=\sum_{\substack{0\le a\le b\le d\\ k_j=1 \text{ for all } a<j\le b}}\frac{(2\pi i)^{b-a+1}}{(b-a+1)!}I_{\mathrm{dch}}(0';1,\overbrace{0,\dots,0}^{k_1-1},\dots,1,\overbrace{0,\dots,0}^{k_a-1};1')\\
&\qquad\times I_{\mathrm{dch}^{-1}}(1';\overbrace{0,\dots,0}^{k_{b+1}-1},1,\dots,\overbrace{0,\dots,0}^{k_d-1}1;0')\\
&=\sum_{\substack{0\le a\le b\le d\\ k_j=1 \text{ for all } a<j\le b}}\frac{(2\pi i)^{b-a+1}}{(b-a+1)!}(-1)^{a+d-b+k_{b+1}+\cdots+k_d}\zeta_{ш}(k_1,\dots,k_a)\\
&\qquad\times \zeta_{ш}(k_d,\dots,k_{b+1})\\
&=(-1)^d 2\pi i\sum_{\substack{0\le a\le b\le d\\ k_j=1 \text{ for all } a<j\le b}}\frac{(-2\pi i)^{b-a}}{(b-a+1)!}(-1)^{k_{b+1}+\cdots+k_d}\zeta_{ш}(k_1,\dots,k_a)\\
&\qquad\times \zeta_{ш}(k_d,\dots,k_{b+1}).
\end{aligned}
$$

Thus the claim is proved. □

Corollary 5. *We have* $\zeta^{RS}(k_1,\dots,k_d)\in\mathcal{Z}[2\pi i]$.

Corollary 6. $\zeta^{RS}(k_1,\dots,k_d)$ *is a lift of* $\zeta^{S}(k_1,\dots,k_d)$ *i.e.,*

$$
\zeta^{RS}(k_1,\dots,k_d)\equiv\sum_{i=0}^{d}(-1)^{k_{i+1}+\cdots+k_d}\zeta_{ш}(k_1,\dots,k_i)\zeta_{ш}(k_d,\dots,k_{i+1})
\pmod{2\pi i\mathcal{Z}[2\pi i]}.
$$

Remark 7. Corollary 6 can also be deduced from the expansion

$$
\Phi_{\mathrm{KZ}}^{-1}e^{2i\pi e_1}\Phi_{\mathrm{KZ}}=1+2i\pi\Phi_{\mathrm{KZ}}^{-1}e_1\Phi_{\mathrm{KZ}}+(2i\pi)^2\Phi_{\mathrm{KZ}}^{-1}\sum_{n\ge2}\frac{(2i\pi)^{n-2}e_1^n}{n!}\Phi_{\mathrm{KZ}}
$$

given in [7, page26] since $\Phi_{\mathrm{KZ}}^{-1}e_1\Phi_{\mathrm{KZ}}$ is the generating function of $\zeta^S_{ш}(\Bbbk):=\zeta^S_{ш}(\Bbbk;0,0)$.

3 Relations of refined symmetric multiple zeta values

In this section, we state the double shuffle relations, the duality, and the reversal formula for the refined symmetric multiple zeta values. For this purpose, we first introduce some notations and algebraic setup.

3.1 Algebraic settings

Let $\mathbb{Q}\langle e_0, e_1\rangle$ be the free non-commutative ring generated by formal symbols e_0 and e_1 over $\mathbb{Q}$. Put

$$\mathfrak{h} := e_0\mathbb{Q}\langle e_0, e_1\rangle \oplus e_1\mathbb{Q}\langle e_0, e_1\rangle \subset \mathbb{Q}\langle e_0, e_1\rangle,$$
$$\mathfrak{h}^0 := e_1\mathbb{Q} \oplus e_1\mathbb{Q}\langle e_0, e_1\rangle e_1.$$

For $k_1, \ldots, k_d \in \mathbb{Z}_{\geq 1}$, define $w(k_1, \ldots, k_d) \in \mathfrak{h}^0$ by

$$w(k_1, \ldots, k_d) = (-1)^d e_1 e_0^{k_1-1} e_1 \cdots e_1 e_0^{k_d-1} e_1.$$

Note that $w(\emptyset) = e_1$ where $\emptyset = ()$ is an empty index, and that the elements $w(k_1, \ldots, k_d)$ with $d \geq 0$ and $k_1, \ldots, k_d \in \mathbb{Z}_{\geq 1}$ form a basis of $\mathfrak{h}^0$. We define a linear map $Z^{RS} : \mathfrak{h} \to \mathbb{C}$ by

$$Z^{RS}(e_{a_1} \cdots e_{a_k}) = \frac{1}{2\pi i} I_\beta(0'; a_1, \ldots, a_k; 0').$$

From the definition, $Z^{RS}(w(k_1, \ldots, k_d)) = \zeta^{RS}(k_1, \ldots, k_d)$.

3.2 Double shuffle relations

We define the shuffle product $⧢ : \mathbb{Q}\langle e_0, e_1\rangle \times \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle e_0, e_1\rangle$ by the recursion

$$u ⧢ 1 = 1 ⧢ u = u,$$
$$e_a u ⧢ e_b u' = e_a(u ⧢ e_b u') + e_b(e_a u ⧢ u'),$$

where $a, b \in \{0, 1\}$ and $u, u' \in \mathbb{Q}\langle e_0, e_1\rangle$, and define the harmonic product $* : \mathfrak{h}^0 \times \mathfrak{h}^0 \to \mathfrak{h}^0$ by

$$e_1 * u = u * e_1 = u,$$

$$\begin{aligned} w(k_1, \ldots, k_a) * w(l_1, \ldots, l_b) = &- e_1 e_0^{k_1-1} \left(w(k_2, \ldots, k_a) * w(l_1, \ldots, l_b)\right) \\ &- e_1 e_0^{l_1-1} \left(w(k_1, \ldots, k_a) * w(l_2, \ldots, l_b)\right) \\ &+ e_1 e_0^{k_1+l_1-1} \left(w(k_2, \ldots, k_a) * w(l_2, \ldots, l_b)\right). \end{aligned}$$

For example, $w(k) * w(l) = w(k, l) + w(l, k) + w(k + l)$.

Theorem 8 (Double shuffle relations for RSMZVs). *We have*

- $Z^{RS}(u ⧢ v) = 2\pi i Z^{RS}(u) Z^{RS}(v)$ *for* $u, v \in \mathfrak{h}$,
- $Z^{RS}(u * v) = Z^{RS}(u) Z^{RS}(v)$ *for* $u, v \in \mathfrak{h}^0$.

The first formula is an immediate consequence of the iterated integral expression of RSMZVs, but the second one is not obvious from the definition. We give a proof of Theorem 8 in Section 4.2 in a more general setting.

Remark 9. In [7, page27], Jarossay also mentioned about the fact that the first formula of the theorem above is an immediate consequence of the iterated integral expression for RSMZVs.

3.3 Duality and reversal formula

We define an automorphism φ and anti-automorphism τ of $\mathbb{Q}\langle e_0, e_1\rangle$ by

$$\varphi(e_0) = e_0 - e_1,\ \varphi(e_1) = -e_1,$$

$$\tau(e_0) = -e_0,\ \tau(e_1) = -e_1.$$

Theorem 10. *We have*

- $Z^{RS}(\varphi(w)) = -\overline{Z^{RS}(w)}$ *for* $w \in \mathfrak{h}^0$,
- $Z^{RS}(\tau(w)) = -\overline{Z^{RS}(w)}$ *for* $w \in \mathfrak{h}$.

Proof. The first formula follows from the Möbius transformation $t \mapsto \frac{t}{t-1}$. The second formula follows from the reversal formula of iterated integrals. □

4 Relation to other versions of symmetric multiple zeta values

For $n \in \mathbb{Z}$, put $\beta_n = \mathrm{dch} \cdot \alpha^n \cdot \mathrm{dch}^{-1} \in \pi_1(\mathbb{C} \setminus \{0,1\}, 0', 0')$. Define a linear map $L_n : \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{C}$ by

$$L_n(e_{a_1} \cdots e_{a_k}) := I_{\beta_n}(0'; a_1, \dots, a_k; 0').$$

For $w \in \mathbb{Q}\langle e_0, e_1\rangle$, let $L(w;T) \in \mathbb{C}[T]$ be the unique polynomial of T such that

$$L_n(w) = L(w; 2\pi i n).$$

We see the existence of such a polynomial as in the proof of Proposition 4 by using the path composition formula. From the definition, for $w \in \mathfrak{h}$ we have

$$Z^{RS}(w) = \frac{1}{2\pi i} L(w; 2\pi i).$$

We can consider many variants of lifts of symmetric multiple zeta values. In this section, we express such variants by using $L(w;T)$.

4.1 Generating functions

For an index $\Bbbk$, we denote by $\zeta_{Ш}(\Bbbk;T) \in \mathbb{R}[T]$ (resp. $\zeta_*(\Bbbk;T) \in \mathbb{R}[T]$) the shuffle (resp. harmonic) regularized multiple zeta values with T, which are characterized by the shuffle (resp. harmonic) product identity and $\zeta_{Ш}(1;T) = \zeta_*(1;T) = T$. For $d \ge 0$ and $k_1, \dots, k_d \in \mathbb{Z}_{\ge 1}$, we put

$$\zeta^S_{Ш}(k_1, \dots, k_d; T_1, T_2) := \sum_{i=0}^{d} (-1)^{k_d + \cdots + k_{i+1}} \zeta_{Ш}(k_1, \dots, k_i; T_1) \zeta_{Ш}(k_d, \dots, k_{i+1}; T_2),$$

$$\zeta_*^S(k_1,\dots,k_d;T_1,T_2) := \sum_{i=0}^{d}(-1)^{k_d+\cdots+k_{i+1}}\zeta_*(k_1,\dots,k_i;T_1)\zeta_*(k_d,\dots,k_{i+1};T_2).$$

Let $R=\mathbb{Q}\langle\langle X_0,X_1\rangle\rangle$. Put $\Gamma_1(t)=\exp(\sum_{k=2}^{\infty}\frac{\zeta(k)}{k}(-t)^k)\in\mathbb{R}[[t]]$. Define an anti-automorphism $\epsilon : R\to R$ by $\epsilon(X_a)=-X_a$. Put

$$\begin{aligned}
\Phi_{ш}(T) &:= \sum_{k=0}^{\infty}\sum_{a_1,\dots,a_k\in\{0,1\}} I_{\mathrm{dch}}(0';a_1,\dots,a_k;1')X_{a_1}\cdots X_{a_k}\exp(-TX_1)\\
\Phi_*(T) &:= \Phi_{ш}(T)\Gamma_1(-X_1)^{-1}\\
\Phi_{ш}^S(T_1,T_2) &:= \Phi_{ш}(T_1)X_1\epsilon(\Phi_{ш}(T_2))\\
\Phi_*^S(T_1,T_2) &:= \Phi_*(T_1)X_1\epsilon(\Phi_*(T_2))\\
\Phi^{RS} &:= \sum_{k=1}^{\infty}\sum_{a_1,\dots,a_k\in\{0,1\}} Z^{RS}(e_{a_1}\cdots e_{a_k})X_{a_1}\cdots X_{a_k}\\
\Phi^{L}(T) &:= \sum_{k=0}^{\infty}\sum_{a_1,\dots,a_k\in\{0,1\}} L(e_{a_1}\cdots e_{a_k};T)X_{a_1}\cdots X_{a_k}.
\end{aligned}$$

We denote by $\mathrm{coeff}(f,X_{a_1}\cdots X_{a_k})$ the coefficient of $X_{a_1}\cdots X_{a_k}$ in f. The following formulas are essentially proved in [5, Proposition 10 and Theorem 1].

$$\begin{aligned}
\mathrm{coeff}(\Phi_{ш}(T),X_1X_0^{k_1-1}\cdots X_1X_0^{k_d-1}) &= (-1)^d\zeta_{ш}(k_1,\dots,k_d;T)\\
\mathrm{coeff}(\Phi_*(T),X_1X_0^{k_1-1}\cdots X_1X_0^{k_d-1}) &= (-1)^d\zeta_*(k_1,\dots,k_d;T).
\end{aligned}$$

Thus from the definition, we have

$$\begin{aligned}
\mathrm{coeff}(\Phi_{ш}^S(T_1,T_2),X_1X_0^{k_1-1}\cdots X_1X_0^{k_d-1}X_1) &= (-1)^d\zeta_{ш}^S(k_1,\dots,k_d;T_1,T_2)\\
\mathrm{coeff}(\Phi_*^S(T_1,T_2),X_1X_0^{k_1-1}\cdots X_1X_0^{k_d-1}X_1) &= (-1)^d\zeta_*^S(k_1,\dots,k_d;T_1,T_2).
\end{aligned}$$

Theorem 11. *We have*

$$\begin{aligned}
\Phi_{ш}^S(T_1,T_2) &= \frac{d}{dT}\Phi^L(T)\Big|_{T=-T_1+T_2},\\
\Phi_*^S(T_1,T_2) &= \frac{\Phi^L(\pi i-T_1+T_2)-\Phi^L(-\pi i-T_1+T_2)}{2\pi i},\\
\Phi^{RS} &= \frac{\Phi^L(2\pi i)-\Phi^L(0)}{2\pi i}\qquad (=\frac{\Phi^L(2\pi i)-1}{2\pi i}),\\
\Phi^{RS} &= \frac{1}{2\pi i}\int_0^{2\pi i}\Phi_{ш}^S(0,T)dT,\\
\Phi^{RS} &= \Phi_*^S(-\frac{\pi i}{2},\frac{\pi i}{2}).
\end{aligned}\tag{4.1}$$

Proof. It is enough to prove the first and second formulas since the third formula is obvious from the definition and the fourth and fifth formulas are consequences of first three formulas. From the path composition formula, we have

$$\Phi^L(T) = \Phi_{ш}(0)\exp(TX_1)\epsilon(\Phi_{ш}(0)). \tag{4.2}$$

Thus the first and second formulas are proved as follows. For the first, we compute

$$\begin{aligned}\Phi^S_{ш}(T_1,T_2) =& \Phi_{ш}(T_1)X_1\epsilon(\Phi_{ш}(T_2))\\ =& \Phi_{ш}(0)\exp(-T_1X_1)X_1\epsilon(\Phi_{ш}(0)\exp(-T_2X_1))\\ =& \Phi_{ш}(0)\exp((-T_1+T_2)X_1)X_1\epsilon(\Phi_{ш}(0))\\ =& \frac{d}{dT}\Phi^L(T)\bigg|_{T=-T_1+T_2}.\end{aligned}$$

Here, we have used $\Phi_{ш}(T) = \Phi_{ш}(0)\exp(-TX_1)$ for the second equality and (4.2) for the last equality. For the second one, we compute similarly using (4.2) and the classical formula for the gamma function as

$$\begin{aligned}\Phi^S_*(T_1,T_2) &= \Phi_*(T_1)X_1\epsilon(\Phi_*(T_2))\\ &= \Phi_{ш}(0)\Gamma_1(-X_1)^{-1}\exp(-T_1X_1)X_1\\ &\qquad\times\epsilon\left(\Phi_{ш}(0)\Gamma_1(-X_1)^{-1}\exp(-T_2X_1)\right)\\ &= \Phi_{ш}(0)\Gamma_1(-X_1)^{-1}\Gamma_1(X_1)^{-1}X_1\exp(-(T_1-T_2)X_1)\epsilon(\Phi_{ш}(0))\\ &= \Phi_{ш}(0)\frac{\sin(\pi X_1)}{\pi}\exp((-T_1+T_2)X_1)\epsilon(\Phi_{ш}(0))\\ &= \frac{\Phi^L(\pi i-T_1+T_2)-\Phi^L(-\pi i-T_1+T_2)}{2\pi i}.\end{aligned}$$

□

Comparing the coefficients of the identities in the theorem, we get the following corollary.

Corollary 12. *For* $\Bbbk=(k_1,\dots,k_d)\in(\mathbb{Z}_{\geq1})^d$, *we have*

$$\begin{aligned}\zeta^S_{ш}(\Bbbk;T_1,T_2) &= \frac{d}{dT}L(w(\Bbbk);T)\bigg|_{T=-T_1+T_2},\\ \zeta^S_*(\Bbbk;T_1,T_2) &= \frac{L(w(\Bbbk);\pi i-T_1+T_2)-L(w(\Bbbk);-\pi i-T_1+T_2)}{2\pi i}\\ \zeta^{RS}(\Bbbk) &= \frac{1}{2\pi i}\int_0^{2\pi i}\zeta^S_{ш}(\Bbbk;0,T)dT,\\ \zeta^{RS}(\Bbbk) &= \zeta^S_*(\Bbbk;-\frac{\pi i}{2},\frac{\pi i}{2}).\end{aligned} \tag{4.3}$$

Remark 13. In [1], Bachmann, Takeyama and Tasaka introduced complex numbers $\xi(\Bbbk)$ as limits of certain finite multiple harmonic q-series. They also prove the equation

$$\xi(k_d,\dots,k_1)=\sum_{a=0}^{d}(-1)^{k_d+\cdots+k_{a+1}}\zeta_*(k_1,\dots,k_a;-\frac{\pi i}{2})\zeta_*(k_d,\dots,k_{a+1};\frac{\pi i}{2})$$
$$(=\zeta_*^S(k_1,\dots,k_d;-\frac{\pi i}{2},\frac{\pi i}{2}))$$

(see [1, Theorem 2.10, (2.18)]). Thus we have

$$\xi(k_d,\dots,k_1)=\zeta^{RS}(k_1,\dots,k_d)$$

from the last formula of Corollary 12.

4.2 Proof of the double shuffle relations

Proposition 14. *We have*

- $L(u ⧢ v;T)=L(u;T)L(v;T)$ *for all* $u,v\in\mathbb{Q}\langle e_0,e_1\rangle$,
- $\tilde{L}(u*v;T)=\frac{1}{2\pi i}\tilde{L}(u;T)\tilde{L}(v;T)$ *for all* $u,v\in\mathfrak{h}^0$ *where we put* $\tilde{L}(u;T):=L(u;T+\pi i)-L(u;T-\pi i)$.

Proof. The first formula follows from the shuffle product formula for iterated integrals. Define the harmonic coproduct $\Delta:\mathfrak{h}^0\to\mathfrak{h}^0\otimes\mathfrak{h}^0$ by

$$\Delta(w(k_1,\dots,k_d)):=\sum_{i=0}^{d}w(k_1,\dots,k_i)\otimes w(k_{i+1},\dots,k_d).$$

Then $(\mathfrak{h}^0,*,\Delta)$ is a commutative Hopf algebra (see [4, Theorem 3.1]). We define $f:\mathfrak{h}^0\to\mathbb{R}[T_1,T_2]$ by $f(u)=\frac{1}{2\pi i}\tilde{L}(u;T)$. Since $f(w(\Bbbk))=\zeta_*^S(\Bbbk;T_1,T_2)$ by (4.3), f coincides with the composite map

$$\mathfrak{h}^0\xrightarrow{\Delta}\mathfrak{h}^0\otimes\mathfrak{h}^0\xrightarrow{g\otimes h}\mathbb{R}[T_1]\otimes\mathbb{R}[T_2]\xrightarrow{a\otimes b\mapsto ab}\mathbb{R}[T_1,T_2]$$

where g,h are defined by

$$g(w(k_1,\dots,k_d))=\zeta_*(k_1,\dots,k_d;T_1),$$
$$h(w(k_1,\dots,k_d))=(-1)^{k_d+\cdots+k_1}\zeta_*(k_d,\dots,k_1;T_2).$$

Since $(\mathfrak{h}^0,*,\Delta)$ is a Hopf algebra and g,h are ring homomorphisms from $(\mathfrak{h}^0,*)$ to $\mathbb{R}[T_1]$ or $\mathbb{R}[T_2]$, we have

$$f(u*v)=f(u)f(v),$$

which is equivalent to the second formula of the proposition. □

Proof of Theorem 8. By putting $T=2\pi i$ in the first formula of Proposition 14, we obtain the first formula of Theorem 8. By putting $T=\pi i$ in the second formula of Proposition 14, we obtain the second formula of Theorem 8. □

Remark 15. It is also possible to prove the second formula of Theorem 8 by the identity $\xi(k_d,\dots,k_1)=\zeta^{\mathrm{RS}}(k_1,\dots,k_d)$ and the harmonic product formula of the cyclotomic analogue of finite multiple zeta values ([1, (3.4)]) since $z_n(\Bbbk;e^{2\pi i/n})$ in their paper satisfy $\lim_{n\to\infty}(1-e^{2\pi i/n})z_n(\Bbbk;e^{2\pi i/n})=0$.

5 Complementary results and a conjecture

5.1 The space generated by RSMZVs

For an index $\Bbbk=(k_1,\dots,k_d)$, we call $k_1+\cdots+k_d$ the weight of $\Bbbk$. For $k\in\mathbb{Z}$, we denote by $\mathcal{Z}_k$ (resp. $\mathcal{Z}_k^{RS}$) the subspace of $\mathbb{C}$ over $\mathbb{Q}$ generated by all MZVs (resp. RSMZVs) of weight k indices, i.e., we put

$$\mathcal{Z}_k := \langle \zeta_{\sqcup\!\sqcup}(k_1,\dots,k_d)\mid d\in\mathbb{Z}_{\ge0},\ k_1,\dots,k_d\in\mathbb{Z}_{\ge1},\ k_1+\cdots+k_d=k\rangle_{\mathbb{Q}},$$
$$\mathcal{Z}_k^{RS} := \left\langle \zeta^{RS}(k_1,\dots,k_d)\mid d\in\mathbb{Z}_{\ge0},\ k_1,\dots,k_d\in\mathbb{Z}_{\ge1},\ k_1+\cdots+k_d=k\right\rangle_{\mathbb{Q}}.$$

Proposition 16. *For $k\in\mathbb{Z}$, we have*

$$\mathcal{Z}_k^{RS}=\mathcal{Z}_k\oplus 2\pi i\mathcal{Z}_{k-1}.$$

We need some lemma to prove this proposition.

Proof. Since $\mathcal{Z}_k^{RS}\subset\mathcal{Z}_k\oplus 2\pi i\mathcal{Z}_{k-1}$ from Proposition 4, it is enough to prove that

$$\mathcal{Z}_k\oplus 2\pi i\mathcal{Z}_{k-1}\subset\mathcal{Z}_k^{RS}.$$

We prove the proposition by induction on k. The case $k<0$ is trivial. Assume that $\mathcal{Z}_{k-1}^{RS}=\mathcal{Z}_{k-1}\oplus 2\pi i\mathcal{Z}_{k-2}$. Let x be an element of $\mathcal{Z}_k$. From the theorem of Yasuda ([10, Theorem 6.1]), there exists $y\in\mathcal{Z}_k^{RS}$ such that $x-y\in 2\pi i\mathcal{Z}_{k-1}\oplus(2\pi i)^2\mathcal{Z}_{k-2}$. Thus

$$\frac{x-y}{2\pi i}\in\mathcal{Z}_{k-1}\oplus 2\pi i\mathcal{Z}_{k-2}=\mathcal{Z}_{k-1}^{RS}.$$

From the special case of the shuffle product formula

$$Z^{RS}(e_1\sqcup\!\sqcup u)=2\pi i Z^{RS}(u)\quad(u\in\mathfrak{h}),$$

we have $x-y\in 2\pi i\mathcal{Z}_{k-1}^{RS}\subset\mathcal{Z}_k^{RS}$. Thus $x=(x-y)+y\in\mathcal{Z}_k^{RS}$ and the claim is proved. ☐

It is conjectured by Zagier that

$$\dim_{\mathbb{Q}}\mathcal{Z}_k\overset{?}{=}d_k \tag{5.1}$$

where $(d_k)_k$ are integers defined by

$$d_k=\begin{cases}0 & k<0\\ 1 & k=0\\ d_{k-2}+d_{k-3} & k>0.\end{cases}$$

Therefore, from Proposition 16, the conjectural dimension of $\mathcal{Z}_k^{RS}$ is given by

$$\dim_{\mathbb{Q}} \mathcal{Z}_k^{RS} \overset{?}{=} d_k + d_{k-1}.$$

5.2 Comparison of the shuffle relations of RSMZVs and Kaneko-Zagier's shuffle relations for SMZVs

We define $Z^S : \mathfrak{h}^0 \to \mathcal{Z}/\zeta(2)\mathcal{Z}$ by $Z^S(w(k_1,\dots,k_d)) := \zeta^S(k_1,\dots,k_d)$. Put $\tilde{Z}^S(u) = Z^S(ue_1)$ and $\bar{u} = -e_1\tau(u)e_1^{-1}$ for $u \in \mathbb{Q} \oplus e_1\mathbb{Q}\langle e_0, e_1\rangle$. The following relations of SMZVs were already known.

Proposition 17 ([9],[11, Corollary 6.1.5]). *$Z^S(u) * Z^S(v) = Z^S(u)Z^S(v)$ for $u, v \in \mathfrak{h}^0$.*

Proposition 18 ([6],[9],[11, Theorem 6.3.4]). *$\tilde{Z}^S(u \sqcup\!\sqcup v) = \tilde{Z}^S(u\bar{v})$ or equivalently $Z^S((u \sqcup\!\sqcup v)e_1) = Z^S(ue_1\epsilon(v))$ for $u, v \in \mathbb{Q} \oplus e_1\mathbb{Q}\langle e_0, e_1\rangle$.*

Proposition 19 ([6, Corollaire 1.12]). *$Z^S(\varphi(u)) = -Z^S(u)$ for $u \in \mathfrak{h}^0$.*

Proposition 20 ([9],[11, Theorem 6.3.4]). *$Z^S(\epsilon(u)) = -Z^S(u)$ for $u \in \mathfrak{h}^0$.*

On the other hand, we proved the following relations of RSMZVs in this paper.

(i) $Z^{RS}(u) * Z^{RS}(v) = Z^{RS}(u)Z^{RS}(v)$ for $u, v \in \mathfrak{h}^0$ (Theorem 8).

(ii) $Z^{RS}(u \sqcup\!\sqcup v) = 2\pi i Z^{RS}(u)Z^{RS}(v)$ for $u, v \in \mathfrak{h}$ (Theorem 8).

(iii) $Z^{RS}(\varphi(u)) = -\overline{Z^{RS}(u)}$ for $u \in \mathfrak{h}^0$ (Theorem 10).

(iv) $Z^{RS}(\epsilon(u)) = -\overline{Z^{RS}(u)}$ for $u \in \mathfrak{h}$ (Theorem 10).

Now Propositions 17, 19 and 20 are immediate consequences of (i), (iii) and (iv) respectively. However the relation of Proposition 18 and (ii) is not obvious. The purpose of this section is to deduce Proposition 18 from (ii). First, we show that Corollary 5 can be extended as follows.

Lemma 21. *For $u \in \mathfrak{h}$, we have*

$$Z^{RS}(u) \in \mathcal{Z}[2\pi i].$$

Proof. The claim follows from the identity

$$\Phi^{RS} = \Phi_{\sqcup\!\sqcup}(0)\frac{\exp(2\pi i X_1) - 1}{2\pi i}\epsilon(\Phi_{\sqcup\!\sqcup}(0)),$$

which is a consequence of (4.1) and (4.2). □

Lemma 22. *We denote by $\mathfrak{h} \sqcup\!\sqcup \mathfrak{h}$ the subspace of $\mathfrak{h}$ spanned by $\{u \sqcup\!\sqcup v \mid u, v \in \mathfrak{h}\}$. Then for all $u, v \in \mathbb{Q}\langle e_0, e_1\rangle$ and $a \in \{0, 1\}$, we have*

$$(u \sqcup\!\sqcup v)e_a - ue_a\epsilon(v) \in \mathfrak{h} \sqcup\!\sqcup \mathfrak{h}.$$

Proof. It is enough to consider only the case where v is a monomial $e_{b_1}\cdots e_{b_n}$. Then we have

$$(u ⧢ v)e_a - ue_a\epsilon(v) = -\sum_{i=1}^{n}(u ⧢ e_{b_{i+1}}\cdots e_{b_n})e_a ⧢ \epsilon(e_{b_1}\cdots e_{b_i}) \in \mathfrak{h} ⧢ \mathfrak{h}. \quad \square$$

Proof of Proposition 18 using (ii). Let $u,v \in \mathbb{Q}\oplus e_1\mathbb{Q}\langle e_0,e_1\rangle$. From Lemma 22, we have

$$(u ⧢ v)e_1 - ue_1\epsilon(v) \in \mathfrak{h} ⧢ \mathfrak{h}.$$

Hence from (ii) and Lemma 21, we have

$$Z^{RS}((u ⧢ v)e_1 - ue_1\epsilon(v)) \in 2\pi i\mathcal{Z}[2\pi i].$$

Therefore, from Corollary 6, we have

$$Z^{S}((u ⧢ v)e_1 - ue_1\epsilon(v)) = 0.$$

Thus Proposition 18 is proved. $\square$

5.3 The size of the double shuffle relations of RSMZVs

We define a grading $\mathfrak{h} = \oplus_{k=-1}^{\infty}\mathfrak{h}_k$ by $\mathfrak{h}_k = \oplus_{a_1,\dots,a_{k+1}\in\{0,1\}}\mathbb{Q}e_{a_1}\cdots e_{a_{k+1}}$. We put $\mathfrak{h}_k^0 := \mathfrak{h}_k \cap \mathfrak{h}^0$. From Theorem 8, we have

$$D(u,v,w) := u * (v ⧢ w) - v ⧢ (u * w) \in \ker Z^{RS}$$

for $u,v,w \in \mathfrak{h}^0$. For example

$$D(e_1^2, e_1, e_1) = 2w(2) + w(1,1) \in \ker Z^{RS}.$$

Conjecture 23. *All $\mathbb{Q}$-linear relations of RSMZVs are generated by $D(u,v,w)$, i.e., the space $\ker Z^{RS} \subset \mathfrak{h}^0$ is linearly spanned by*

$$\{D(u,v,w) \mid u,v,w \in \mathfrak{h}^0\}.$$

If we assume Zagier's conjecture (5.1), the above conjecture is equivalent to the following conjecture.

Conjecture 24. *For $k \ge 1$, we have*

$$\dim_{\mathbb{Q}}\left\langle D(u,v,w)\,\middle|\, {\scriptstyle a+b+c=k-1, \atop (u,v,w)\in\mathfrak{h}_a^0\times\mathfrak{h}_b^0\times\mathfrak{h}_c^0}\right\rangle_{\mathbb{Q}} \ge 2^{k-1} - d_k - d_{k-1}.$$

For $u,v,w \in \mathfrak{h}^0$, we put

$$\begin{aligned} D'(u,v,w) :&= D(w,v,u) - D(u,v,w) + D(u,w,v) \\ &= w * (u ⧢ v) - w ⧢ (u * v). \end{aligned}$$

For $u \in \mathfrak{h}^a, v \in \mathfrak{h}^b$ and $k \geq 1$, we denote by $E_k(u,v)$ (resp. $E'_k(v,w)$) the subspaces of $\mathfrak{h}^0_k$ spanned by $\{D(u,v,w) \mid w \in \mathfrak{h}^0_{k-a-b-1}\}$ (resp. $\{D'(u,v,w) \mid w \in \mathfrak{h}^0_{k-a-b-1}\}$). We verified Conjecture 24 up to $k=16$ by numerical computation. More precisely, we checked that the dimension of the $\mathbb{Q}$-linear subspace spanned by

$$E_k(e_1^2, e_1) \cup E_k(e_1^2, e_1 e_0 e_1^2) \cup E'_k(e_1, e_1) \cup E'_k(e_1^2, e_1) \cup E'_k(e_1^2, e_1^2)$$

is greater than or equal to $2^{k-1} - d_k - d_{k-1}$ for each $1 \leq k \leq 16$.

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