EXPLICIT DOUBLE SHUFFLE RELATIONS AND A GENERALIZATION OF EULER'S DECOMPOSITION FORMULA

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Abstract. We give an explicit formula for the shuffle relation in a general double shuffle framework that specializes to double shuffle relations of multiple zeta values and multiple polylogarithms. As an application, we generalize the well-known decomposition formula of Euler that expresses the product of two Riemann zeta values as a sum of double zeta values to a formula that expresses the product of two multiple polylogarithm values as a sum of other multiple polylogarithm values.

Keywords: Euler's decomposition formula, multiple zeta values, multiple polylogarithm values, double shuffle relation.

1. Introduction

Euler's decomposition formula is the equation

$$\zeta(r)\zeta(s) = \sum_{k=0}^{s-1} \binom{r+k-1}{k} \zeta(r+k, s-k) + \sum_{k=0}^{r-1} \binom{s+k-1}{k} \zeta(s+k, r-k), \quad r, s \geqslant 2, \tag{1}$$

expressing the product of two Riemann zeta values as a sum of double zeta values

$$\zeta(s_1, s_2) := \sum_{n_1 > n_2 \geqslant 1} \frac{1}{n_1^{s_1} n_2^{s_2}}.$$

This formula, together with Euler's sum formula

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

are the two classical identities on double zeta values before the multiple zeta values (MZVs)

$$\zeta(s_1, \cdots, s_k) := \sum_{n_1 > \cdots > n_k \geqslant 1} \frac{1}{n_1^{s_1} \cdots n_k^{s_k}}$$

were introduced in the 1990s [23, 38]. Since then MZVs have been studied quite intensively involving many areas of mathematics and physics, from mixed Tate motives [11, 37] to quantum field theory [9].

A major aspect of these studies is finding algebraic and linear relations among MZVs, such as Euler's formulas. Euler's sum formula was soon generalized to MZVs [23, 17, 39] as the well-known sum formula, followed by quite a few other generalizations [7, 12, 21, 26, 28, 31, 32, 33, 34]. To the contrary, no generalizations of Euler's decomposition formula to MZVs, either proved or conjectured, have been given even though Euler's formula has been revisited recently [1, 4, 13] and generalized to the product of two q-zeta values [8, 40]. In our view this situation is due to the lack of a suitable context in which a generalization of Euler's formula makes sense, and the correct language and tools to formulate and prove such a generalization.

In this paper we generalize Euler's decomposition formula in two directions, from the product of one variable functions to that of multiple variables and from multiple zeta values to multiple polylogarithms. We achieve this by viewing Euler's decomposition formula as a special instance of the important double shuffle relation to motivate our generalizations, establishing a general framework of shuffle and quasi-shuffle algebras to formulate these generalizations and applying a suitable interpretation of the shuffle relation to prove these generalizations.

To motivate our approach, we illustrate the relationship between Euler's decomposition formula and the double shuffle relations of MZVs. Because of the representations of an MZV as an iterated sum and as an iterated integral, the multiplication of two MZVs can be expressed in two ways as the sum of other MZVs, one way following the **quasi-shuffle (stuffle) relation** and the other way following the **shuffle relation**. The combination of these two relations (called the **double shuffle relations**) generates an extremely rich family of relations among MZVs. In fact, as a conjecture, all relations among MZVs can be derived from these relations and their degenerated forms, altogether called the **extended double shuffle relations** [27, 35]. A consequence of this conjecture is the irrationality of $\zeta(n)$ for all odd integers $n \geqslant 3$.

Naturally, determining all the extended double shuffle relations is challenging and the efforts have utilized a wide range of methods. One difficulty is that the shuffle relations have not been explicitly formulated in terms of the MZVs. For example, to determine the double shuffle relation from multiplying two Riemann zeta values $\zeta(r)$ and $\zeta(s)$, $r, s \geqslant 2$, one uses their sum representations and easily gets the quasi-shuffle relation

$$\zeta(r)\zeta(s) = \zeta(r, s) + \zeta(s, r) + \zeta(r + s). \tag{2}$$

On the other hand, to get their shuffle relation, one first needs to use their integral representations to express $\zeta(r)$ and $\zeta(s)$ as iterated integrals of dimensions r and s, respectively. One then uses the shuffle relation to express the product of these two iterated integrals as a sum of $\binom{r+s}{r}$ iterated integrals of dimension $r + s$. Finally, these last iterated integrals are translated back to MZVs and give the shuffle relation of $\zeta(r)\zeta(s)$. *We observe that the explicit shuffle relation in this case is precisely the decomposition formula of Euler in Eq. (1).* See also [4]. Then together with Eq. (2), we have the double shuffle relation from $\zeta(r)$ and $\zeta(s)$. For the applications of the double shuffle relation in this special case, we refer the reader to [13] on the connection of double zeta values with modular forms, and to [34] on weighted sum formula of double zeta values.

In general, even though the computation of the shuffle relation can be performed recursively for any given pair of MZVs, an explicit formula, naturally a generalization of Euler's decomposition formula, is missing so far. As the above example demonstrates, such an explicit formula not only provides an effective way to evaluate the shuffle relation, but also is important in the theoretical study of MZVs, especially the double shuffle relations. There are several families of special values in addition to MZVs, such as the alternating Euler sums [2], the polylogarithms and multiple polylogarithms [3, 14], especially at roots of unity [35], where the double shuffle relations are also studied [5, 35, 41], but are less understood. Such an explicit formula for these values should also be useful to their study.

Thus we have obtained a suitable context of double shuffle relations to look for a generalization of Euler's decomposition formula. It is still challenging to predict and prove such a generalization using the standard notion of shuffles. Instead we work with the alternative characterization of a shuffle as a suitable pair of order preserving injective maps, allowing us to establish explicit shuffle formulas for the product of any two MZVs, alternating Euler sums and multiple polylogarithms, thereby achieving our generalizations of Euler's formula mentioned above.

As a concrete example, we obtain, for integers $r_1, s_1 \geqslant 2$ and $s_2 \geqslant 1$,

$$\zeta(r_1)\,\zeta(s_1,s_2) = \sum_{\substack{t_1\geqslant 2, t_2\geqslant 1\\ t_1+t_2=r_1+s_1}} \binom{t_1-1}{r_1-1}\zeta(t_1,t_2,s_2) + \sum_{\substack{t_1\geqslant 2, t_2,t_3\geqslant 1\\ t_1+t_2+t_3\\ =r_1+s_1+s_2}} \binom{t_1-1}{s_1-1}\left[\binom{t_2-1}{s_2-t_3}+\binom{t_2-1}{s_2-1}\right]\zeta(t_1,t_2,t_3). \tag{3}$$

As another instance, for integers $r_1, s_1 \geqslant 2$ and $r_2, s_2 \geqslant 1$, we have

$$\begin{aligned}
&\zeta(r_1,r_2)\,\zeta(s_1,s_2)\\
&= \sum_{\substack{t_1\geqslant 2, t_2,t_3\geqslant 1\\ t_1+t_2+t_3=r_1+r_2+s_1}} \binom{t_1-1}{r_1-1}\binom{t_2-1}{r_2-1}\zeta(t_1,t_2,t_3,s_2) + \sum_{\substack{t_1\geqslant 2, t_2,t_3\geqslant 1\\ t_1+t_2+t_3=r_1+s_1+s_2}} \binom{t_1-1}{s_1-1}\binom{t_2-1}{s_2-1}\zeta(t_1,t_2,t_3,r_2)\\
&\quad + \sum_{\substack{t_1\geqslant 2, t_2,t_3,t_4\geqslant 1\\ t_1+t_2+t_3+t_4=\\ r_1+r_2+s_1+s_2}} \left[\binom{t_1-1}{r_1-1}\binom{t_2-1}{t_1+t_2-r_1-s_1}\left(\binom{t_3-1}{s_2-t_4}+\binom{t_3-1}{s_2-1}\right)\right.\\
&\qquad\qquad \left. +\binom{t_1-1}{s_1-1}\binom{t_2-1}{t_1+t_2-r_1-s_1}\left(\binom{t_3-1}{r_2-t_4}+\binom{t_3-1}{r_2-1}\right)\right]\zeta(t_1,t_2,t_3,t_4).
\end{aligned} \tag{4}$$

We hope this framework can be further extended to deal with other generalizations of multiple zeta values that have emerged recently, such as the multiple q-zeta values [7, 40] and renormalized MZVs [21, 22, 30].

The organization of the paper is as follows. In Section 2, we first describe the algebraic framework of double shuffle algebras. We then give our main formula in two variations (Theorem 2.1 and Theorem 2.2). Theorem 2.1 is more general and easier to prove. Theorem 2.2 is more convenient for applications to multiple polylogarithm values and MZVs (Corollary 2.4 and Corollary 2.5). There we also provide some examples. The proofs of the main theorems are quite long. So several lemmas are first proved in Section 3. Then these lemmas are applied in Section 4 to prove the main formula by induction. As an appendix, Section 5 includes a shuffle product formulation of the main formula.

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2. The main theorems, applications and examples

We first set up in Section 2.1 a framework of general double shuffles to give a uniform formulation of the double shuffle relations for multiple zeta values, alternating Euler sums and multiple polylogarithms. We then state in Section 2.2 our main formula in two variations in this framework. Applications to the aforementioned special values are presented in Section 2.3. Computations in low dimensions and examples are provided in Section 2.4.

2.1. **The general double shuffle framework.** We formulate the framework to state our main theorems in Section 2.2. See Section 2.3 for the concrete cases that have been considered before [3, 14, 24, 35, 41].

We first introduce some notations. For any set Y, denote $M(Y)$ for the free monoid generated by Y. Let $\mathcal{H}(Y)$ be the free abelian group $\mathbb{Z}M(Y)$ with $M(Y)$ as a basis but without considering the product from the monoid $M(Y)$. When $\mathcal{H}(Y)$ is equipped with an associative multiplication $\circ$, we use $\mathcal{H}^{\circ}(Y)$ to denote the algebra $(\mathcal{H}(Y), \circ)$.

Let G be a given set. Define

$$\overline{G} = \{x_0\} \cup \{x_b \mid b \in G\}$$

to be the set of symbols indexed by the disjoint set $\{0\} \sqcup G$. Then the shuffle algebra [29, 36] generated by $\overline{G}$ is

$$\mathcal{H}^{ш}(\overline{G}) := (\mathbb{Z}M(\overline{G}), ш) \tag{5}$$

where the shuffle product $ш$ is defined recursively by

$$(a_1\mathfrak{a}) ш (b_1\mathfrak{b}) = a_1(\mathfrak{a} ш (b_1\mathfrak{b})) + b_1((a_1\mathfrak{a}) ш \mathfrak{b}), a_1, b_1 \in \overline{G}, \mathfrak{a}, \mathfrak{b} \in M(\overline{G})$$

with the convention that $1 ш \mathfrak{b} = \mathfrak{b} = \mathfrak{b} ш 1$ for $\mathfrak{b} \in M(\overline{G})$. Define the subalgebra

$$\mathcal{H}^{ш}_1(\overline{G}) := \mathbb{Z} \oplus (\oplus_{b\in G} \mathcal{H}^{ш}(\overline{G})x_b) \subseteq \mathcal{H}^{ш}(\overline{G}). \tag{6}$$

For the given set G, let $\widehat{G}$ be the set product

$$\widehat{G} := \mathbb{Z}_{\geqslant 1} \times G = \{w := \left[\begin{smallmatrix} s \\ b \end{smallmatrix}\right] \mid s \in \mathbb{Z}_{\geqslant 1}, b \in G\}.$$

We will denote the non-unit elements in the free monoid $M(\widehat{G})$ by vectors

$$\vec{v} := [v_1, \cdots, v_k] = \left[\begin{smallmatrix} s_1, \cdots, s_k \\ b_1, \cdots, b_k \end{smallmatrix}\right] = \left[\begin{smallmatrix} \vec{s} \\ \vec{b} \end{smallmatrix}\right] \in \widehat{G}^k$$

and denote $[v_1, [v_2, \cdots, v_k]] = [v_1, v_2, \cdots, v_k]$. Consider the free abelian group

$$\mathcal{H}(\widehat{G}) := \mathbb{Z}M(\widehat{G}) = \bigoplus_{\vec{v}\in\widehat{G}^k, k\geqslant 0} \mathbb{Z}\vec{v}, \quad \widehat{G}^0 = \{1\}.$$

As in the case of the shuffle algebra from MZVs, elements of $\mathcal{H}^{ш}_1(\overline{G})$ of the form

$$x_0^{s_1-1}x_{b_1}x_0^{s_2-1}x_{b_2}\cdots x_0^{s_k-1}x_{b_k}, \quad s_i \geqslant 1, b_i \in G, 1 \leqslant i \leqslant k, k \geqslant 1,$$

together with 1, form a basis of $\mathcal{H}^{ш}_1(\overline{G})$. Since $\mathcal{H}(\widehat{G})$ with the concatenation product is the free non-commutative algebra generated by $\widehat{G}$, there is a natural linear bijection

$$\rho : \mathcal{H}^{ш}_1(\overline{G}) \to \mathcal{H}(\widehat{G}), \quad x_0^{s_1-1}x_{b_1}\cdots x_0^{s_k-1}x_{b_k} \leftrightarrow \left[\begin{smallmatrix} s_1, & s_2, & \cdots, & s_k \\ b_1, & b_2, & \cdots, & b_k \end{smallmatrix}\right], \quad 1 \leftrightarrow 1. \tag{7}$$

Through ρ, the shuffle product $ш$ on $\mathcal{H}^{ш}_1(\overline{G})$ defines a product on $\mathcal{H}(\widehat{G})$ by

$$\vec{\mu} ш_\rho \vec{v} := \rho(\rho^{-1}(\vec{\mu}) ш \rho^{-1}(\vec{v})), \quad \vec{\mu}, \vec{v} \in \mathcal{H}(\widehat{G}). \tag{8}$$

Following our notations, we use $\mathcal{H}^{ш_\rho}(\widehat{G})$ to denote this algebra.

Now assume that G is a multiplicative abelian group. Equip $\widehat{G} = \mathbb{Z}_{\geqslant 1} \times G$ with the abelian semigroup structure by the component multiplication: $\left[\begin{smallmatrix} s_1 \\ z_1 \end{smallmatrix}\right] \cdot \left[\begin{smallmatrix} s_2 \\ z_2 \end{smallmatrix}\right] = \left[\begin{smallmatrix} s_1+s_2 \\ z_1 z_2 \end{smallmatrix}\right]$. Then we define the quasi-shuffle algebra [25] on $\widehat{G}$ to be

$$\mathcal{H}^*(\widehat{G}) := (\mathbb{Z}M(\widehat{G}), *) \tag{9}$$

where the multiplication $*$ is defined by the recursion

$$[\mu_1, \vec{\mu}\,'] * [\nu_1, \vec{\nu}\,'] = [\mu_1, (\vec{\mu}\,' * [\nu_1, \vec{\nu}\,'])] + [\nu_1, [\mu_1, \vec{\mu}\,'] * \vec{\nu}\,'] + [(\mu_1 \cdot \nu_1), \vec{\mu}\,' * \vec{\nu}\,'],$$

$\mu_1, \nu_1 \in \widehat{G}, \vec{\mu}\,', \vec{\nu}\,' \in M(\widehat{G})$, with the initial condition that $1 * \vec{\nu} = \vec{\nu} = \vec{\nu} * 1$ for $\vec{\nu} \in M(\widehat{G})$. See [18, 19, 25] for its explicit description and its structure.

We define a linear bijection

$$\theta : \mathcal{H}^*(\widehat{G}) \to \mathcal{H}^*(\widehat{G}), \quad \left[\begin{smallmatrix} s_1, \cdots, s_k \\ b_1, \cdots, b_k \end{smallmatrix}\right] \mapsto \left[\begin{smallmatrix} s_1,\ s_2, \cdots,\ s_k \\ \frac{1}{b_1}, \frac{b_1}{b_2}, \cdots, \frac{b_{k-1}}{b_k} \end{smallmatrix}\right] \tag{10}$$

whose inverse is given by

$$\theta^{-1} : \mathcal{H}^*(\widehat{G}) \to \mathcal{H}^*(\widehat{G}), \quad \left[\begin{smallmatrix} s_1, \cdots, s_k \\ z_1, \cdots, z_k \end{smallmatrix}\right] \mapsto \left[\begin{smallmatrix} s_1,\ s_2, \cdots,\ s_k \\ \frac{1}{z_1}, \frac{1}{z_1 z_2}, \cdots, \frac{1}{z_1 \cdots z_k} \end{smallmatrix}\right] \tag{11}$$

Note that the action of θ is defined by an action on the second row of elements in $\mathcal{H}^*(\widehat{G})$ which is again denoted by θ:

$$\theta(b_1, \cdots, b_k) = \left(\frac{1}{b_1}, \frac{b_1}{b_2}, \cdots, \frac{b_{k-1}}{b_k}\right). \tag{12}$$

The composition of ρ and θ gives a natural bijection of abelian groups (but *not* as algebras)

$$\eta : \mathcal{H}^{ш}_1(\overline{G}) \to \mathcal{H}^*(\widehat{G}), \quad x_0^{s_1-1} x_{b_1} \cdots x_0^{s_k-1} x_{b_k} \leftrightarrow \left[\begin{smallmatrix} s_1,\ s_2,\ \cdots,\ s_k \\ \frac{1}{b_1},\ \frac{b_1}{b_2},\ \cdots,\ \frac{b_{k-1}}{b_k} \end{smallmatrix}\right] \tag{13}$$

whose inverse is given by $\left[\begin{smallmatrix} s_1, \cdots, s_k \\ z_1, \cdots, z_k \end{smallmatrix}\right] \mapsto x_0^{s_1-1} x_{z_1^{-1}} x_0^{s_2-1} x_{(z_1 z_2)^{-1}} \cdots x_0^{s_k-1} x_{(z_1 \cdots z_k)^{-1}}$.

Through η, the shuffle product ш on $\mathcal{H}^{ш}_1(\overline{G})$ transports to a product $ш_\eta$ on $\mathcal{H}(\widehat{G})$, resulting a commutative algebra $\mathcal{H}^{ш_\eta}(\widehat{G}) = (\mathcal{H}(\widehat{G}), ш_\eta)$. More precisely, for $\vec{\mu}, \vec{\nu} \in \mathcal{H}(\widehat{G})$,

$$\vec{\mu} ш_\eta \vec{\nu} := \eta(\eta^{-1}(\vec{\mu})\, ш\, \eta^{-1}(\vec{\nu})). \tag{14}$$

Then we have the following commutative diagram of commutative algebras:

$$\begin{tikzcd} \mathcal{H}^{ш}_0(\overline{S^1}) \arrow[r, "\rho"] \arrow[rr, bend left, "\eta"] & \mathcal{H}^{ш_\rho}_0(\widehat{S}^1) \arrow[r, "\theta"] & \mathcal{H}^{ш_\eta}_0(\widehat{S}^1) \end{tikzcd} \tag{15}$$

The purpose of this paper is to give an explicit formula for $\vec{\mu} ш_\eta \vec{\nu}$ (Theorem 2.2) which naturally gives shuffle formulas for MZVs, MPVs and alternating Euler sums. However, as we will see later, for the proof of this formula, it is more convenient to work with its variation (Theorem 2.1) for the product $ш_\rho$ since it is more compatible with the module structure on $\mathcal{H}^*(\widehat{G})$. This approach also allows us to obtain a formula without requiring that G is a group, further extending its potential of applications that will be discussed in a future work.

2.2. **The statement of the main theorems.** We first introduce some notations. For positive integers k and ℓ, denote $[k]=\{1,\cdots,k\}$ and $[k+1,k+\ell]=\{k+1,\cdots,k+\ell\}$. Define

$$\mathfrak{I}_{k,\ell}=\left\{(\varphi,\psi)\,\middle|\,\begin{array}{l}\varphi:[k]\to[k+\ell],\psi:[\ell]\to[k+\ell] \text{ are order preserving}\\ \text{injective maps and } \mathrm{im}(\varphi)\sqcup\mathrm{im}(\psi)=[k+\ell]\end{array}\right\} \tag{16}$$

Let $\vec{a}\in G^k$, $\vec{b}\in G^\ell$ and $(\varphi,\psi)\in\mathfrak{I}_{k,\ell}$. We define $\vec{a}\,Ш_{(\varphi,\psi)}\vec{b}$ to be the vector whose ith component is

$$(\vec{a}\,Ш_{(\varphi,\psi)}\vec{b})_i=\left\{\begin{array}{ll} a_j & \text{if } i=\varphi(j)\\ b_j & \text{if } i=\psi(j)\end{array}\right. = a_{\varphi^{-1}(i)}b_{\psi^{-1}(i)},\quad 1\leqslant i\leqslant k+\ell, \tag{17}$$

with the convention that $a_\emptyset=b_\emptyset=1$.

Let $\vec{r}=(r_1,\cdots,r_k)\in\mathbb{Z}_{\geqslant1}^k$, $\vec{s}=(s_1,\cdots,s_\ell)\in\mathbb{Z}_{\geqslant1}^\ell$ and $\vec{t}=(t_1,\cdots,t_{k+\ell})\in\mathbb{Z}_{\geqslant1}^{k+\ell}$ with $|\vec{r}|+|\vec{s}|=|\vec{t}|$. Here $|\vec{r}|=r_1+\cdots+r_k$ and similarly for $|\vec{s}|$ and $|\vec{t}|$. Denote $R_i=r_1+\cdots+r_i$ for $i\in[k]$, $S_i=s_1+\cdots+s_i$ for $i\in[\ell]$ and $T_i=t_1+\cdots+t_i$ for $i\in[k+\ell]$. For $i\in[k+\ell]$, define

$$h_{(\varphi,\psi),i}=h_{(\varphi,\psi),(\vec{r},\vec{s}),i}=\left\{\begin{array}{ll} r_j & \text{if } i=\varphi(j)\\ s_j & \text{if } i=\psi(j)\end{array}\right. = r_{\varphi^{-1}(i)}s_{\psi^{-1}(i)}, \tag{18}$$

with the convention that $r_\emptyset=s_\emptyset=1$.

With these notations, we define

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)=\left\{\begin{array}{ll} \binom{t_i-1}{h_{(\varphi,\psi),i}-1} & \begin{array}{l}\text{if } i=1, \text{if } i-1,i\in\mathrm{im}(\varphi)\\ \text{or if } i-1,i\in\mathrm{im}(\psi),\end{array}\\ \begin{array}{l}\binom{t_i-1}{T_i-R_{|\varphi^{-1}([i])|}-S_{|\psi^{-1}([i])|}}\\ =\binom{t_i-1}{\sum_{j=1}^{i}t_j-\sum_{j=1}^{i}h_{(\varphi,\psi),j}}\end{array} & \text{otherwise.}\end{array}\right. \tag{19}$$

Denote

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}:=\prod_{i=1}^{k+\ell}c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)=\prod_{j=1}^{k}c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(\varphi(j))\prod_{j=1}^{\ell}c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(\psi(j)). \tag{20}$$

Now we can state the first variation of our main formula.

Theorem 2.1. *Let k,ℓ be positive integers. Let G be a set and let $\mathcal{H}^{Ш_\rho}(\widehat{G})=(\mathcal{H}(\widehat{G}),Ш_\rho)$ be the algebra defined by Eq. (8). Then for $\left[\begin{array}{c}\vec{r}\\ \vec{a}\end{array}\right]\in\widehat{G}^k$ and $\left[\begin{array}{c}\vec{s}\\ \vec{b}\end{array}\right]\in\widehat{G}^\ell$ in $\mathcal{H}^{Ш_\rho}(\widehat{G})$, we have*

$$\begin{aligned}\left[\begin{array}{c}\vec{r}\\ \vec{a}\end{array}\right]Ш_\rho\left[\begin{array}{c}\vec{s}\\ \vec{b}\end{array}\right] &= \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}\\ \vec{t}\in\mathbb{Z}_{\geqslant1}^{k+\ell},|\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}\left[\begin{array}{c}\vec{t}\\ \vec{a}\,Ш_{(\varphi,\psi)}\vec{b}\end{array}\right]\\ &= \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}\\ \vec{t}\in\mathbb{Z}_{\geqslant1}^{k+\ell},|\vec{t}|=|\vec{r}|+|\vec{s}|}}\left(\prod_{i=1}^{k+\ell}c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)\right)\left[\begin{array}{c}\vec{t}\\ \vec{a}\,Ш_{(\varphi,\psi)}\vec{b}\end{array}\right],\end{aligned} \tag{21}$$

where $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)$ is given in Eq. (19) and $\vec{a}\,Ш_{(\varphi,\psi)}\vec{b}$ is given in Eq. (17).

For the purpose of applications to MZVs and multiple polylogarithms, we give an equivalent form of Theorem 2.1 under the condition that G is an abelian group. For $\vec{w} \in G^k$ and $\vec{z} \in G^\ell$, we define

$$(\vec{w}\star_{(\varphi,\psi)}\vec{z})_i = \begin{cases} w_j & \text{if } i = \varphi(j) \text{ and either } i = 1 \text{ or } i-1 \in \operatorname{im}(\varphi), \\ z_j & \text{if } i = \psi(j) \text{ and either } i = 1 \text{ or } i-1 \in \operatorname{im}(\varphi), \\ \frac{w_1\cdots w_j}{z_1\cdots z_{i-j}} & \text{if } i = \varphi(j) \text{ and } i-1 \in \operatorname{im}(\psi), \\ \frac{z_1\cdots z_j}{w_1\cdots w_{i-j}} & \text{if } i = \psi(j) \text{ and } i-1 \in \operatorname{im}(\varphi). \end{cases} \tag{22}$$

Theorem 2.2. *Let k,ℓ be positive integers. Let G be an abelian group and let $\mathcal{H}^{ш_\eta}(\widehat{G}) = (\mathcal{H}(\widehat{G}), ш_\eta)$ be the algebra defined by Eq. (14). Then for $\left[\begin{smallmatrix}\vec{r}\\ \vec{w}\end{smallmatrix}\right] \in \widehat{G}^k$ and $\left[\begin{smallmatrix}\vec{s}\\ \vec{z}\end{smallmatrix}\right] \in \widehat{G}^\ell$ in $\mathcal{H}^{ш_\eta}(\widehat{G})$, we have*

$$\begin{aligned} \left[\begin{smallmatrix}\vec{r}\\ \vec{w}\end{smallmatrix}\right] ш_\eta \left[\begin{smallmatrix}\vec{s}\\ \vec{z}\end{smallmatrix}\right] &= \sum_{\substack{(\varphi,\psi)\in\mathcal{I}_{k,\ell}\\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell},|\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \left[\begin{smallmatrix}\vec{t}\\ \vec{w}\star_{(\varphi,\psi)}\vec{z}\end{smallmatrix}\right] \\ &= \sum_{\substack{(\varphi,\psi)\in\mathcal{I}_{k,\ell}\\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell},|\vec{t}|=|\vec{r}|+|\vec{s}|}} \left(\prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)\right) \left[\begin{smallmatrix}\vec{t}\\ \vec{w}\star_{(\varphi,\psi)}\vec{z}\end{smallmatrix}\right], \end{aligned} \tag{23}$$

where $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)$ is given in Eq. (19) and $\vec{w}\star_{(\varphi,\psi)}\vec{z}$ is given in Eq. (22).

We will next give applications and examples of Theorem 2.2 in Section 2.3 and Section 2.4. Theorem 2.2 will be shown to follow from Theorem 2.1 in Section 4.1, and Theorem 2.1 will be proved in Section 4.2. Preparational lemmas will be given in Section 3.

2.3. **Applications.** In this section, Theorem 2.2 is specialized to give formulas for multiple zeta values, alternating Euler sums and multiple polylogarithms. We start with multiple polylogarithms and then specialize further to MZVs and alternating Euler sums. In Section 2.4 we demonstrate how to apply these formulas by computing examples in low dimensions.

2.3.1. *Multiple polylogarithms.* A **multiple polylogarithm value (**MPV**)** [3, 14, 15] is defined by

$$\operatorname{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k) := \sum_{n_1>\cdots>n_k\geqslant 1} \frac{z_1^{n_1}\cdots z_k^{n_k}}{n_1^{s_1}\cdots n_k^{s_k}} \tag{24}$$

where $|z_i| \leqslant 1$, $s_i \in \mathbb{Z}_{\geqslant 1}$, $1 \leqslant i \leqslant k$, and $(s_1, z_1) \neq (1, 1)$. When $z_i = 1, 1 \leqslant i \leqslant k$, we obtain the multiple zeta values $\zeta(s_1,\cdots,s_k)$ that we will consider in Section 2.3.2. More generally, the special cases when z_i are roots of unity have been studied [3, 6, 15, 35] in connection with high cyclotomic theory, mixed motives and combinatorics, and have been found in the computations of Feynman diagrams [10].

With the notation of [3], we have

$$\begin{aligned} \operatorname{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k) = \lambda\left(\begin{matrix} s_1,\cdots,s_k\\ b_1,\cdots,b_k\end{matrix}\right) &:= \sum_{n_1>n\cdots>n_k\geqslant 1} \frac{(\frac{1}{b_1})^{n_1}(\frac{b_1}{b_2})^{n_2}\cdots(\frac{b_{k-1}}{b_k})^{n_k}}{n_1^{s_1}n_2^{s_2}\cdots n_k^{s_k}}, \\ \text{where } (b_1,\cdots,b_k) = \theta^{-1}(z_1,\cdots,z_k) &= (z_1^{-1},(z_1z_2)^{-1},\cdots,(z_1\cdots z_k)^{-1}). \end{aligned} \tag{25}$$

Here θ is as defined in Eq. (12).

The product of two sums representing two MPVs is a $\mathbb{Z}$-linear combination of other such sums. So the $\mathbb{Z}$-linear span of these values is an algebra which we denote by

$$\mathbf{MPV} = \mathbb{Z}\{\mathrm{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k) \mid s_i \in \mathbb{Z}_{\geqslant 1}, |z_i| \leqslant 1, (s_1,z_1) \neq (1,1)\}.$$

In the framework of Section 2.1 and Section 2.2, take G to be the multiplicative abelian group $S^1 := \{z \in \mathbb{C}^\times \mid |z| = 1\}$, and consider the subalgebra

$$\mathcal{H}_0^*(\widehat{S^1}) := \mathbb{Z} \oplus \Big(\bigoplus_{\left[\begin{smallmatrix} s_1 \\ z_1 \end{smallmatrix}\right] \neq \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]} \mathbb{Z}\left[\begin{smallmatrix} s_1, s_2, \cdots, s_k \\ z_1, z_2, \cdots, z_k \end{smallmatrix}\right] \Big) \subseteq \mathcal{H}^*(\widehat{S^1}).$$

Then $\mathcal{H}^*(\widehat{G})$ coincides with the quasi-shuffle (stuffle) algebra [15, 35] encoding MPVs, and the multiplication rule of two MPVs according to their sum representations in Eq. (24) follows from the fact that the linear map

$$\mathrm{Li}^* : \mathcal{H}_0^*(\widehat{S^1}) \to \mathbf{MPV}, \quad \left[\begin{smallmatrix} s_1, \cdots, s_k \\ z_1, \cdots, z_k \end{smallmatrix}\right] \mapsto \mathrm{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k)$$

is an algebra homomorphism.

We also consider the shuffle algebra $\mathcal{H}^{Ш}(\overline{S^1})$ and its subalgebras

$$\begin{aligned} \mathcal{H}_0^{Ш}(\overline{S^1}) &:= \mathbb{Z} \oplus \big(\oplus_{a,b \in \{0\} \cup S^1, a \neq 1, b \neq 0}\, x_a \mathcal{H}^{Ш}(\overline{S^1}) x_b \big) \\ &\subseteq \mathcal{H}_1^{Ш}(\overline{S^1}) := \mathbb{Z} \oplus \big(\oplus_{b \in S^1}\, \mathcal{H}^{Ш}(\overline{S^1}) x_b \big) \subseteq \mathcal{H}^{Ш}(\overline{S^1}). \end{aligned}$$

They agree with the shuffle algebras [14, 35] encoding MPVs through their integral representations [3, 14, 35]

$$\mathrm{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k) = \int_0^1 \int_0^{u_1} \cdots \int_0^{u_{|\vec{s}|-1}} \frac{du_1}{f_1(u_1)} \cdots \frac{du_{|\vec{s}|}}{f_{|\vec{s}|}(u_{|\vec{s}|})}. \tag{26}$$

Here

$$f_j(u_j) = \begin{cases} (z_1 \cdots z_i)^{-1} - u_j & \text{if } j = s_1 + \cdots + s_i, 1 \leqslant i \leqslant k, \\ u_j & \text{otherwise.} \end{cases}$$

It takes a simpler form in terms of $\lambda\left(\begin{smallmatrix} s_1, \cdots, s_k \\ b_1, \cdots, b_k \end{smallmatrix} \right)$ thanks to Eq. (25):

$$\lambda\left(\begin{matrix} s_1, \cdots, s_k \\ b_1, \cdots, b_k \end{matrix} \right) = \int_0^1 \int_0^{u_1} \cdots \int_0^{u_{|\vec{s}|-1}} \frac{du_1}{g_1(u_1)} \cdots \frac{du_{|\vec{s}|}}{g_{|\vec{s}|}(u_{|\vec{s}|})}, \tag{27}$$

as commented in the introduction of [3]. Here

$$g_j(u_j) = \begin{cases} b_i - u_j & \text{if } j = s_1 + \cdots + s_i, 1 \leqslant i \leqslant k, \\ u_j & \text{otherwise.} \end{cases}$$

The multiplication rule of two MPVs according to their integral representations in Eq. (27) follows from the algebra homomorphism [3, §5.4]

$$\mathrm{Li}^{Ш} : \mathcal{H}_0^{Ш}(\overline{S^1}) \to \mathbf{MPV}, \quad x_0^{s_1-1} x_{b_1} \cdots x_0^{s_k-1} x_{b_k} \mapsto \lambda\left(\begin{matrix} s_1, \cdots, s_k \\ b_1, \cdots, b_k \end{matrix} \right).$$

The algebra isomorphism $\rho : \mathcal{H}^{\shuffle}_1(\overline{S^1}) \to \mathcal{H}^{\shuffle_\rho}(\widehat{S^1})$ in Eq. (7) restricts to an algebra isomorphism

$$\rho : \mathcal{H}^{\shuffle}_0(\overline{S^1}) \to \mathcal{H}^{\shuffle_\rho}_0(\widehat{S^1}), \quad x_0^{s_1-1}x_{b_1}\cdots x_0^{s_k-1}x_{b_k} \leftrightarrow \left[\begin{smallmatrix} s_1, & s_2, & \cdots, & s_k \\ b_1, & b_2, & \cdots, & b_k \end{smallmatrix}\right].$$

Similarly the algebra isomorphisms $\eta : \mathcal{H}^{\shuffle}(\overline{S^1}) \to \mathcal{H}^{\shuffle_\eta}(\widehat{S^1})$ in Eq. (13) and $\theta : \mathcal{H}^{\shuffle_\rho}(\widehat{S^1}) \to \mathcal{H}^{\shuffle_\eta}(\widehat{S^1})$ in Eq. (10) restrict to algebra isomorphisms

$$\eta : \mathcal{H}^{\shuffle}_0(\overline{S^1}) \to \mathcal{H}^{\shuffle_\eta}_0(\widehat{S^1}), \quad \theta : \mathcal{H}^{\shuffle_\rho}_0(\widehat{S^1}) \to \mathcal{H}^{\shuffle_\eta}_0(\widehat{S^1}).$$

Define

$$\mathrm{Li}^{\shuffle_\rho} : \mathcal{H}^{\shuffle_\rho}_0(\widehat{S^1}) \to \mathbf{MPV}, \quad \left[\begin{smallmatrix} s_1,\cdots,s_k \\ b_1,\cdots,b_k \end{smallmatrix}\right] \mapsto \lambda\begin{pmatrix} s_1,\cdots,s_k \\ b_1,\cdots,b_k \end{pmatrix} \tag{28}$$

and

$$\mathrm{Li}^{\shuffle_\eta} : \mathcal{H}^{\shuffle_\eta}_0(\widehat{S^1}) \to \mathbf{MPV}, \quad \left[\begin{smallmatrix} s_1,\cdots,s_k \\ z_1,\cdots,z_k \end{smallmatrix}\right] \mapsto \mathrm{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k). \tag{29}$$

Then we can organize these maps into the following commutative diagram extending the commutative diagram in (15):

$$\begin{tikzcd}
\mathcal{H}^{\shuffle}_0(\overline{S^1}) \arrow[r, "\rho"] \arrow[rr, bend left, "\eta"] \arrow[dr, "\mathrm{Li}^{\shuffle}"'] & \mathcal{H}^{\shuffle_\rho}_0(\widehat{S^1}) \arrow[r, "\theta"] \arrow[d, "\mathrm{Li}^{\shuffle_\rho}"] & \mathcal{H}^{\shuffle_\eta}_0(\widehat{S^1}) \arrow[dl, "\mathrm{Li}^{\shuffle_\eta}"] \\
& \mathbf{MPV} &
\end{tikzcd}$$

where the commutativity of the left triangle follows from the definitions of the maps and that of the right triangle follows from Eq. (25). Since $\mathrm{Li}^{\shuffle}$ is an algebra homomorphism and ρ and η are algebra isomorphisms, it follows that $\mathrm{Li}^{\shuffle_\rho}$ and $\mathrm{Li}^{\shuffle_\eta}$ are also algebra homomorphisms.

Therefore, applying $\mathrm{Li}^{\shuffle_\rho}$ to the two sides of Eq. (21) in Theorem 2.1, we obtain

Corollary 2.3. *Let k, ℓ be positive integers. Let $\vec{r} \in \mathbb{Z}^k_{\geqslant 1}$ and $\vec{s} \in \mathbb{Z}^\ell_{\geqslant 1}$. Let $\vec{a} = (a_1, \cdots, a_k) \in (S^1)^k$ and $\vec{b} = (b_1, \cdots, b_\ell) \in (S^1)^\ell$ such that $\left[\begin{smallmatrix} r_1 \\ a_1 \end{smallmatrix}\right] \neq \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} s_1 \\ b_1 \end{smallmatrix}\right] \neq \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$.*

$$\lambda\begin{pmatrix} \vec{r} \\ \vec{a} \end{pmatrix} \lambda\begin{pmatrix} \vec{s} \\ \vec{b} \end{pmatrix} = \sum_{\vec{t} \in \mathbb{Z}^{k+\ell}_{\geqslant 1}, |\vec{t}| = |\vec{r}| + |\vec{s}|} \sum_{(\varphi,\psi) \in \mathfrak{I}_{k,\ell}} \Big(\prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) \Big) \lambda\begin{pmatrix} \vec{t} \\ \vec{a} \shuffle_{(\varphi,\psi)} \vec{b} \end{pmatrix}.$$

where $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)$ is given in Eq. (19) and $\vec{a} \shuffle_{(\varphi,\psi)} \vec{b}$ is given in Eq. (17).

Similarly, applying $\mathrm{Li}^{\shuffle_\eta}$ to the two sides of Eq. (23) in Theorem 2.2, we obtain

Corollary 2.4. *Let k, ℓ be positive integers. Let $\vec{r} \in \mathbb{Z}^k_{\geqslant 1}$ and $\vec{s} \in \mathbb{Z}^\ell_{\geqslant 1}$. Let $\vec{w} = (w_1, \cdots, w_k) \in (S^1)^k$ and $\vec{z} = (z_1, \cdots, z_\ell) \in (S^1)^\ell$ such that $\left[\begin{smallmatrix} r_1 \\ w_1 \end{smallmatrix}\right] \neq \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} s_1 \\ z_1 \end{smallmatrix}\right] \neq \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$. Then*

$$\mathrm{Li}_{\vec{r}}(\vec{w})\,\mathrm{Li}_{\vec{s}}(\vec{z}) = \sum_{\vec{t} \in \mathbb{Z}^{k+\ell}_{\geqslant 1}, |\vec{t}| = |\vec{r}| + |\vec{s}|} \sum_{(\varphi,\psi) \in \mathfrak{I}_{k,\ell}} \Big(\prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) \Big) \mathrm{Li}_{\vec{t}}(\vec{w} \star_{(\varphi,\psi)} \vec{z})$$

where $c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i)$ is given in Eq. (19) and $\vec{w}\star_{(\varphi,\psi)}\vec{z}$ is given in Eq. (22).

See Section 2.4 for examples in low dimensions.

2.3.2. *Multiple zeta values and alternating Euler sums.* Taking $z_i = 1, 1 \leqslant i \leqslant r$, in $\mathrm{Li}_{s_1,\cdots,s_k}(z_1,\cdots,z_k)$ defined in Eq. (24) and the corresponding integral representation in Eq. (26), we obtain the MZV and its integral representation:

$$\begin{aligned}\zeta(s_1,\cdots,s_k) :&= \sum_{n_1>\cdots>n_k\geqslant 1} \frac{1}{n_1^{s_1}\cdots n_k^{s_k}}\\ &= \int_0^1\int_0^{u_1}\cdots\int_0^{u_{|\vec{s}|-1}} \frac{du_1}{f_1(u_1)}\cdots\frac{du_{|\vec{s}|}}{f_{|\vec{s}|}(u_{|\vec{s}|})}\end{aligned}$$

for integers $s_i \geqslant 1$ and $s_1 > 1$. Here

$$f_j(u_j) = \begin{cases} 1-u_j & \text{if } j = s_1, s_1+s_2,\cdots,s_1+\cdots+s_k,\\ u_j & \text{otherwise.}\end{cases}$$

This is also the case when $G = \{1\}$ in our framework in Section 2.1 and 2.2. Then we can identify $\widehat{G}$ with $\mathbb{Z}_{\geqslant 1}$ and denote $\vec{v} = [\begin{smallmatrix} s_1,\cdots,s_k \\ z_1,\cdots,z_k\end{smallmatrix}] = [\begin{smallmatrix} s_1,\cdots,s_k \\ 1,\cdots,1\end{smallmatrix}]$ by $\mathfrak{z} = \mathfrak{z}_{s_1}\cdots\mathfrak{z}_{s_k}$. Then $\mathcal{H}^*(\widehat{G})$ coincides with the quasi-shuffle algebra $\mathcal{H}^*$ encoding MZVs [25, 27] through the identification $\mathfrak{z}_{s_1}\cdots\mathfrak{z}_{s_k} \leftrightarrow z_{s_1}\cdots z_{s_k}$. We will use $\mathfrak{z}_{s_1}\cdots\mathfrak{z}_{s_k}$ in place of $z_{s_1}\cdots z_{s_k}$ to avoid confusion with the vector $(z_1,\cdots,z_k)$ in $\vec{v}$. $\mathcal{H}^*$ contains the subalgebra

$$\mathcal{H}_0^* := \mathbb{Z}\oplus\mathbb{Z}\{\mathfrak{z}_{s_1}\cdots\mathfrak{z}_{s_k} \,\big|\, s_i\geqslant 1, s_1>1, 1\leqslant i\leqslant k, k\geqslant 1\}.$$

Likewise the shuffle algebra $\mathcal{H}^{ш}(\overline{G})$, when $G = \{1\}$, coincides with the shuffle algebra $\mathcal{H}^{ш}$ [24, 27] encoding MZVs, and there are subalgebras

$$\mathcal{H}_0^{ш} := \mathbb{Z}\oplus x_0\mathcal{H}^{ш}x_1 \subseteq \mathcal{H}_1^{ш} := \mathbb{Z}\oplus\mathcal{H}^{ш}x_1 \subseteq \mathcal{H}^{ш},$$

where $\mathcal{H}_1^{ш}$ coincides with $\mathcal{H}_1^{ш}(\widehat{G})$ defined in Eq. (6). The natural isomorphism $\eta : \mathcal{H}_1^{ш} \to \mathcal{H}^*$ of abelian groups in Eq. (13) restricts to an isomorphism of abelian groups

$$\eta : \mathcal{H}_0^{ш} \to \mathcal{H}_0^*, \quad x_0^{s_1-1}x_1\cdots x_0^{s_k-1}x_1 \leftrightarrow \mathfrak{z}_{s_1}\cdots\mathfrak{z}_{s_k}.$$

With the notation $\mathfrak{z}' ш_\eta \mathfrak{z}'' := \eta(\eta^{-1}(\mathfrak{z}') ш \eta^{-1}(\mathfrak{z}''))$ from Eq. (14), the **double shuffle relation** of MZVs is simply the ideal generated by the set

$$\{\mathfrak{z}' ш_\eta \mathfrak{z}'' - \mathfrak{z}' * \mathfrak{z}'' \mid \mathfrak{z}', \mathfrak{z}'' \in \mathcal{H}_0^*\}$$

and the **extended double shuffle relation** of MZVs [27] is the ideal generated by the set

$$\{\mathfrak{z}' ш_\eta \mathfrak{z}'' - \mathfrak{z}' * \mathfrak{z}'',\ \mathfrak{z}_1 ш_\eta \mathfrak{z}'' - \mathfrak{z}_1 * \mathfrak{z}'' \mid \mathfrak{z}', \mathfrak{z}'' \in \mathcal{H}_0^*\}.$$

While the product $\mathfrak{z}' * \mathfrak{z}''$ simply follows from the quasi-shuffle relation, the evaluation of $\mathfrak{z}' ш_\eta \mathfrak{z}''$ involves first pulling $\mathfrak{z}'$ and $\mathfrak{z}''$ back to $\mathcal{H}_0^{ш}$ by η, then expressing the shuffle product $\eta(\mathfrak{z}') ш \eta(\mathfrak{z}'')$ as a linear combination of words in $M(x_0, x_1)$, and then sending the result forward to $\mathcal{H}_0^*$ by η. While this process can be defined recursively (see Proposition 4.3), the explicit formula is found only in special cases, such as when $\mathfrak{z}' = \mathfrak{z}_r, \mathfrak{z}'' = \mathfrak{z}_s$ are both of dimension one. As we have discussed in the Introduction, the explicit formula in this case is Euler's formula in Eq. (1).

Our Theorem 2.2 provides an explicit formula for $ш_\eta$ and hence for the shuffle product of MZVs in the full generality.

Corollary 2.5. *Let $\vec{r} \in \mathbb{Z}^k_{\geqslant 1}$ and $\vec{s} \in \mathbb{Z}^\ell_{\geqslant 1}$ with $r_1, s_1 \geqslant 2$. Then*

$$\zeta(\vec{r})\,\zeta(\vec{s}) = \sum_{\vec{t}\in\mathbb{Z}^{k+\ell}_{\geqslant 1}, |\vec{t}|=|\vec{r}|+|\vec{s}|} \Big(\sum_{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}} \prod_{i=1}^{k+\ell} c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i) \Big) \zeta(\vec{t})$$

where $c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i)$ is given in Eq. (19).

See Section 2.4 for its specialization to Euler's decomposition formula and other special cases.

Proof. Since $\zeta(\vec{r}) = \mathrm{Li}_{\vec{r}}(\vec{w})$ and $\zeta(\vec{s}) = \mathrm{Li}_{\vec{s}}(\vec{z})$ where the vectors $\vec{w}$ and $\vec{z}$ have 1 as the components, the vectors $\vec{w}\star_{(\varphi,\psi)}\vec{z}$ also have 1 as their components and thus are independent of the choice of $(\varphi,\psi) \in \mathfrak{I}_{k,\ell}$. Then the corollary follows Corollary 2.4. $\square$

Between the case of MZVs and the case of MPVs, there is the case of **alternating Euler sums**, defined by

$$\zeta(s_1, \cdots, s_k; \sigma_1, \cdots, \sigma_k) := \sum_{n_1>\cdots>n_k\geqslant 1} \frac{\sigma_1^{n_1}\cdots\sigma_k^{n_k}}{n_1^{s_1}\cdots n_k^{s_k}},$$

where $\sigma_i = \pm 1, 1 \leqslant i \leqslant k$. This corresponds to the case when $G = \{\pm 1\}$ in our framework. More generally when G is the group of k-th roots of unity, we have the **multiple polylogarithms at roots of unity** [35]. We will not go into the details, but will give an example in Eq. (30) that generalizes Euler's formula.

2.4. **Examples.** We now consider some special cases of Theorem 2.2, Corollary 2.4 and Corollary 2.5.

2.4.1. *The case of $r = s = 1$.* In this case $\vec{r} = r_1$ and $\vec{s} = s_1$ are positive integers, and $\vec{w} = w_1$ and $\vec{z} = z_1$ are in G. Let $\vec{t} = (t_1, t_2) \in \mathbb{Z}^2_{\geqslant 1}$ with $t_1 + t_2 = r_1 + s_1$. If $(\varphi,\psi) \in \mathfrak{I}_{1,1}$, then either $\varphi(1) = 1$ and $\psi(1) = 2$, or $\psi(1) = 1$ and $\varphi(1) = 2$. If $\varphi(1) = 1$ and $\psi(1) = 2$, then by Eq. (19), we obtain

$$c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(1) = \binom{t_1-1}{r_1-1}, \quad c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(2) = \binom{t_2-1}{t_1+t_2-r_1-s_1} = 1$$

and thus

$$c^{\vec{t},(\varphi,\psi)}_{r_1,s_1} = c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(1)\, c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(2) = \binom{t_1-1}{r_1-1}.$$

By Eq. (22), we have

$$\vec{w}\star_{(\varphi,\psi)}\vec{z} = (w_1, z_1/w_1).$$

If $\psi(1) = 1$ and $\varphi(1) = 2$, then by Eq. (19), we obtain

$$c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(1) = \binom{t_1-1}{s_1-1}, \quad c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(2) = \binom{t_2-1}{t_1+t_2-r_1-s_1} = 1$$

and thus

$$c^{\vec{t},(\varphi,\psi)}_{r_1,s_1} = c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(1)\, c^{\vec{t},(\varphi,\psi)}_{r_1,s_1}(2) = \binom{t_1-1}{s_1-1}.$$

By Eq. (22), we have $\vec{w}\star_{(\varphi,\psi)}\vec{z} = (z_1, w_1/z_1)$. Therefore,

$$\begin{aligned}
\left[\begin{smallmatrix} r_1 \\ w_1 \end{smallmatrix}\right] ш_\eta \left[\begin{smallmatrix} s_1 \\ z_1 \end{smallmatrix}\right] &= \sum_{t_1,t_2\geqslant 1, t_1+t_2=r_1+s_1} \binom{t_1-1}{r_1-1} \left[\begin{smallmatrix} t_1,t_2 \\ w_1, z_1/w_1 \end{smallmatrix}\right] + \sum_{t_1,t_2\geqslant 1, t_1+t_2=r_1+s_1} \binom{t_1-1}{s_1-1} \left[\begin{smallmatrix} t_1,t_2 \\ z_1, w_1/z_1 \end{smallmatrix}\right] \\
&= \sum_{t_1,t_2\geqslant 1, t_1+t_2=r_1+s_1} \binom{t_1-1}{t_1-r_1} \left[\begin{smallmatrix} t_1,t_2 \\ w_1, z_1/w_1 \end{smallmatrix}\right] + \sum_{t_1,t_2\geqslant 1, t_1+t_2=r_1+s_1} \binom{t_1-1}{t_1-s_1} \left[\begin{smallmatrix} t_1,t_2 \\ z_1, w_1/z_1 \end{smallmatrix}\right] \\
&= \sum_{k=0}^{s_1-1} \binom{r_1+k-1}{k} \left[\begin{smallmatrix} r_1+k, s_1-k \\ w_1, z_1/w_1 \end{smallmatrix}\right] + \sum_{k=0}^{r_1-1} \binom{s_1+k-1}{k} \left[\begin{smallmatrix} s_1+k, r_1-k \\ z_1, w_1/z_1 \end{smallmatrix}\right]
\end{aligned}$$

by a change of variables $k = t_1 - r_1$ for the first sum and $k = t_1 - s_1$ for the second sum. Then by Corollary 2.4, we obtain the following relation for double polylogarithms

$$\mathrm{Li}_{r_1}(w_1)\mathrm{Li}_{s_1}(z_1) = \sum_{k=0}^{s_1-1} \binom{r_1+k-1}{k} \mathrm{Li}_{r_1+k, s_1-k}(w_1, z_1/w_1) + \sum_{k=0}^{r_1-1} \binom{s_1+k-1}{k} \mathrm{Li}_{s_1+k, r_1-k}(z_1, w_1/z_1),$$

where $r_1, s_1 \geqslant 1$, $w_1, z_1 \in S^1$ and $(r_1, w_1) \neq (1, 1) \neq (s_1, z_1)$. In the special case when $w_1 = \pm 1$ and $z_1 = \pm 1$, we have the following relation for alternating Euler sums

$$\begin{aligned}
\zeta(r_1; w_1)\zeta(s_1; z_1) &= \sum_{k=0}^{s_1-1} \binom{r_1+k-1}{k} \zeta(r_1 + k, s_1 - k; w_1, z_1/w_1) \\
&\quad + \sum_{k=0}^{r_1-1} \binom{s_1+k-1}{k} \zeta(s_1 + k, r_1 - k; z_1, w_1/z_1),
\end{aligned} \tag{30}$$

when $r_1, s_1 \geqslant 1$ and $(r_1, w_1) \neq (1, 1) \neq (s_1, z_1)$.

Further specializing, when $r_1, s_1 \geqslant 2$ and $w_1 = z_1 = 1$, we obtain the decomposition formula of Euler in Eq. (1).

2.4.2. *The case of* $r = 1, s = 2$. In this case $\left[\begin{smallmatrix} \vec{r} \\ \vec{w} \end{smallmatrix}\right] = \left[\begin{smallmatrix} r_1 \\ w_1 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} \vec{s} \\ \vec{z} \end{smallmatrix}\right] = \left[\begin{smallmatrix} s_1, s_2 \\ z_1, z_2 \end{smallmatrix}\right]$. Let $\vec{t} = (t_1, t_2, t_3) \in \mathbb{Z}^3_{\geqslant 1}$ with $t_1 + t_2 + t_3 = r_1 + s_1 + s_2$. There are 3 pairs (φ, ψ) in $\mathcal{I}_{1,2}$.

When $\varphi(1) = 1$, $\psi(1) = 2$ and $\psi(2) = 3$, by Eq. (19), we have

$$c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(1) = \binom{t_1-1}{r_1-1}, \quad c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(2) = \binom{t_2-1}{t_1+t_2-r_1-s_1}, \quad c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(3) = \binom{t_3-1}{s_2-1}.$$

When the second and the third terms are nonzero, we have $t_1 + t_2 \geqslant r_1 + s_2$ and $t_3 \geqslant s_2$. Then the inequalities must be equalities and we have $c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(2) = c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(3) = 1$. Thus

$$c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}} = c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(1)\, c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(2)\, c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}}(3) = \begin{cases} \binom{t_1-1}{r_1-1}, & \text{if } t_3 = s_2, \\ 0, & \text{otherwise} . \end{cases}$$

By Eq. (22) we have

$$\vec{w}\star_{(\varphi,\psi)}\vec{z} = (w_1, z_1/w_1, z_2).$$

Similarly, when $\varphi(1) = 2$, $\psi(1) = 1$ and $\psi(2) = 3$, we have

$$c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}} = \binom{t_1-1}{s_1-1}\binom{t_2-1}{s_2-t_3}, \quad \vec{w}\star_{(\varphi,\psi)}\vec{z} = (z_1, w_1/z_1, z_1 z_2/w_1),$$

and when $\varphi(1) = 3$, $\psi(1) = 1$ and $\psi(2) = 2$, we have

$$c^{\vec{t},(\varphi,\psi)}_{r_1,\vec{s}} = \binom{t_1-1}{s_1-1}\binom{t_2-1}{s_2-1}, \qquad \vec{w}\star_{(\varphi,\psi)}\vec{z} = (z_1, z_2, w_1/(z_1z_2)).$$

Combining these computations with Corollary 2.4 we obtain, for $r_1, s_1, s_2 \geqslant 1$ and $(r_1, w_1) \neq (1, 1) \neq (s_1, z_1)$,

$$\begin{aligned}\mathrm{Li}_{r_1}(w_1)\,\mathrm{Li}_{s_1,s_2}(z_1, z_2) &= \sum_{\substack{t_1,t_2,t_3\geqslant 1\\ t_1+t_2=r_1+s_1}} \binom{t_1-1}{r_1-1}\mathrm{Li}_{(t_1,t_2,s_2)}(w_1, z_1/w_1, z_2)\\ &\quad + \sum_{\substack{t_1,t_2,t_3\geqslant 1\\ t_1+t_2+t_3\\ =r_1+s_1+s_2}} \Bigg[\binom{t_1-1}{s_1-1}\binom{t_2-1}{s_2-t_3}\mathrm{Li}_{(t_1,t_2,t_3)}(z_1, w_1/z_1, z_1z_2/w_1)\\ &\qquad\qquad + \binom{t_1-1}{s_1-1}\binom{t_2-1}{s_2-1}\mathrm{Li}_{(t_1,t_2,t_3)}(z_1, z_2, w_1/(z_1z_2))\Bigg].\end{aligned}$$

Taking $w_1 = z_1 = z_2 = 1$ (or by Corollary 2.5) we obtain the relation in Eq. (3) among MZVs.

2.4.3. *The case of $r = s = 2$.* In this case $\left[\begin{smallmatrix}\vec{r}\\ \vec{w}\end{smallmatrix}\right] = \left[\begin{smallmatrix}r_1,r_2\\ w_1,w_2\end{smallmatrix}\right]$ and $\left[\begin{smallmatrix}\vec{s}\\ \vec{z}\end{smallmatrix}\right] = \left[\begin{smallmatrix}s_1,s_2\\ z_1,z_2\end{smallmatrix}\right]$. Let $\vec{t} = (t_1, t_2, t_3, t_4) \in \mathbb{Z}^4_{\geqslant 1}$ with $t_1 + t_2 + t_3 + t_4 = r_1 + r_2 + s_1 + s_2$. Then there are $\binom{4}{2} = 6$ choices of $(\varphi, \psi) \in \mathfrak{I}_{2,2}$.

If $\varphi(1) = 1$, $\varphi(2) = 2$, $\psi(1) = 3$ and $\psi(2) = 4$, by Eq. (19), we have

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(1) = \binom{t_1-1}{r_1-1}, \qquad c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(2) = \binom{t_2-1}{r_2-1},$$

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(3) = \binom{t_3-1}{t_1+t_2+t_3-r_1-r_2-s_1} = \binom{t_3-1}{s_2-t_4}, \qquad c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(4) = \binom{t_4-1}{s_2-1}.$$

When the third and fourth terms are nonzero, we have $t_1 + t_2 + t_3 \geqslant r_1 + r_2 + s_1$ and $t_4 \geqslant s_2$. Hence they must be equalities and thus $c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(3) = c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(4) = 1$. Then

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(1)\,c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(2)\,c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(3)\,c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(4) = \begin{cases}\binom{t_1-1}{r_1-1}\binom{t_2-1}{r_2-1}, & \text{if } t_4 = s_2,\\ 0, & \text{otherwise.}\end{cases}$$

Similarly, if $\varphi(1) = 3$, $\varphi(2) = 4$, $\psi(1) = 1$ and $\psi(2) = 2$, then

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = \begin{cases}\binom{t_1-1}{s_1-1}\binom{t_2-1}{s_2-1}, & \text{if } t_4 = r_2,\\ 0, & \text{otherwise.}\end{cases}$$

If $\varphi(1) = 1$, $\varphi(2) = 3$, $\psi(1) = 2$ and $\psi(2) = 4$, then

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = \binom{t_1-1}{r_1-1}\binom{t_2-1}{t_1+t_2-r_1-s_1}\binom{t_3-1}{s_2-t_4}.$$

If $\varphi(1) = 2$, $\varphi(2) = 4$, $\psi(1) = 1$ and $\psi(2) = 3$, then

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = \binom{t_1-1}{s_1-1}\binom{t_2-1}{t_1+t_2-r_1-s_1}\binom{t_3-1}{r_2-t_4}.$$

If $\varphi(1) = 1$, $\varphi(2) = 4$, $\psi(1) = 2$ and $\psi(2) = 3$, then

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = \binom{t_1-1}{r_1-1}\binom{t_2-1}{t_1+t_2-r_1-s_1}\binom{t_3-1}{s_2-1}.$$

If $\varphi(1) = 2$, $\varphi(2) = 3$, $\psi(1) = 1$ and $\psi(2) = 4$, then

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = \binom{t_1-1}{s_1-1}\binom{t_2-1}{t_1+t_2-r_1-s_1}\binom{t_3-1}{r_2-1}.$$

Then from Corollary 2.5, we obtain Eq. (4). We likewise obtain formulas for the products of double multiple polylogarithms and those of double alternating Euler sums.

3. Preparational lemmas

In this section we prove some properties of the coefficients $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}$ in our Theorem 2.1 and Theorem 2.2 in preparation for their proofs in the next section.

We recall some notations from Section 2.2. Let $k, \ell \geqslant 1$, $\vec{r} \in \mathbb{Z}_{\geqslant 1}^k$, $\vec{s} \in \mathbb{Z}_{\geqslant 1}^\ell$, $\vec{t} \in \mathbb{Z}_{\geqslant 1}^{k+\ell}$ with $|\vec{t}| = |\vec{r}| + |\vec{s}|$ and $(\varphi, \psi) \in \mathfrak{I}_{k,\ell}$ be given. For $1 \leqslant i \leqslant k + \ell$, denote

$$h_{(\varphi,\psi),i} = h_{(\varphi,\psi),(\vec{r},\vec{s}),i} = \begin{cases} r_j & \text{if } i = \varphi(j), \\ s_j & \text{if } i = \psi(j). \end{cases} \tag{31}$$

We note that, if we define

$$\varepsilon_{\varphi,\psi}(i) = \begin{cases} 1 & \text{if} \quad i \in \mathrm{im}(\varphi), \\ -1 & \text{if} \quad i \in \mathrm{im}(\psi), \end{cases} \tag{32}$$

then Eq. (19) can be rewritten as

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) = \begin{cases} \dbinom{t_i-1}{h_{(\varphi,\psi),i}-1} & \begin{array}{l}\text{if } i = 1 \\ \text{or if } i \geqslant 2 \text{ and } \varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = 1,\end{array} \\ \dbinom{t_i-1}{\sum\limits_{j=1}^{i} t_j - \sum\limits_{j=1}^{i} h_{(\varphi,\psi),j}} & \text{if } i \geqslant 2 \text{ and } \varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = -1. \end{cases} \tag{33}$$

Also recall

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = \prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i).$$

For the inductive proof to work, we also include the case when one of k or ℓ (but not both) is zero which corresponds to the case when $\vec{\mu}$ or $\vec{\nu} \in \mathcal{H}_0^*(\widehat{G})$ is the empty word 1. We will use the convention that $\mathbb{Z}_{\geqslant 1}^0 = \{\mathbf{e}\}$ and denote $|\mathbf{e}| = 0$. When $k = 0$, $\ell \geqslant 1$, we will also denote $\vec{r} = \mathbf{e}$, denote $\mathbf{f} : [k](= \emptyset) \to [k + \ell] = [\ell]$ and denote $\mathfrak{I}_{0,\ell} = \{(\mathbf{f}, \mathrm{id}_{[\ell]})\}$. Similarly, when $\ell = 0$, $k \geqslant 1$, we denote $\vec{s} = \mathbf{e}$, $\mathbf{f} : [\ell] \to [k + \ell] = [k]$ and $\mathfrak{I}_{k,0} = \{(\mathrm{id}_{[k]}, \mathbf{f})\}$. Then the notations in Eq. (31) – (33) still make sense even if exactly one of k and ℓ is zero. More precisely, when $k = 0$, $\ell \geqslant 1$, we have $h_{(\mathbf{f},\mathrm{id}_{[\ell]}),(\mathbf{e},\vec{s}),i} = s_i$, $\varepsilon_{\mathbf{f},\mathrm{id}_{[\ell]}}(i) = -1, 1 \leqslant i \leqslant \ell$. Also, for any $\vec{s}$ and $\vec{t} \in \mathbb{Z}_{\geqslant 1}^\ell$ with $|\vec{s}| = |\vec{t}|$, we have

$$c_{\mathbf{e},\vec{s}}^{\vec{t},(\mathbf{f},\mathrm{id}_{[\ell]})} = \prod_{i=1}^{\ell} \binom{t_i-1}{s_i-1} = \prod_{i=1}^{\ell} \delta_{s_i}^{t_i}. \tag{34}$$

Similarly, if $\vec{s} = \mathbf{e}$, then for any $\vec{r}, \vec{t} \in \mathbb{Z}_{\geqslant 1}^k$ with $|\vec{r}| = |\vec{t}|$, we have $h_{(\mathrm{id}_{[k]},\mathbf{f}),(\vec{r},\mathbf{e}),i} = r_i$, $\varepsilon_{\mathrm{id}_{[k]},\mathbf{f}}(i) = 1$, $1 \leqslant i \leqslant k$ and

$$c_{\vec{r},\mathbf{e}}^{\vec{t},(\mathrm{id}_{[k]},\mathbf{f})} = \prod_{i=1}^{k} \delta_{r_i}^{t_i}. \tag{35}$$

We first give some conditions for the vanishing of $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}$.

Lemma 3.1. *Let $k, \ell \geqslant 1$. Let $\vec{r} \in \mathbb{Z}_{\geqslant 1}^k$, $\vec{s} \in \mathbb{Z}_{\geqslant 1}^\ell$ and $\vec{t} \in \mathbb{Z}_{\geqslant 1}^{k+\ell}$ with $|\vec{r}| + |\vec{s}| = |\vec{t}|$. Let $(\varphi, \psi) \in \mathfrak{I}_{k,\ell}$. Then $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \neq 0$ if and only if, for $1 \leqslant i \leqslant k + \ell$,*

$$\begin{cases} t_i \geqslant h_{(\varphi,\psi),i}, & \text{if } i = 1 \text{ or if } i \geqslant 2 \text{ and } \varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = 1, \\ \sum\limits_{j=1}^{i} t_j \geqslant \sum\limits_{j=1}^{i} h_{(\varphi,\psi),j} > \sum\limits_{j=1}^{i-1} t_j, & \text{if } i \geqslant 2 \text{ and } \varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = -1. \end{cases}$$

Proof. By definition, $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \neq 0$ if and only if $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) \neq 0$ for every $i \in [k+\ell]$. Also $\binom{a}{b} \neq 0$ if and only if $a \geqslant b \geqslant 0$. Then the lemma follows since

$$\Big(t_i - 1 \geqslant h_{(\varphi,\psi),i} - 1 \geqslant 0\Big) \Leftrightarrow \Big(t_i \geqslant h_{(\varphi,\psi),i} \geqslant 1\Big)$$

and

$$\Big(t_i - 1 \geqslant \sum_{j=1}^{i} t_j - \sum_{j=1}^{i} h_{(\varphi,\psi),i} \geqslant 0\Big) \Leftrightarrow \Big(- \sum_{j=1}^{i-1} t_j > - \sum_{j=1}^{i-1} t_j - 1 \geqslant - \sum_{j=1}^{i} h_{(\varphi,\psi),j} \geqslant - \sum_{j=1}^{i} t_j\Big).$$

□

Lemma 3.2. *Let $k, \ell, \vec{r}, \vec{s}, \vec{t}$ be as in Lemma 3.1.*

(a) *Let $(\varphi, \psi) \in \mathfrak{I}_{k,\ell}$. If $\varphi(1) = 1$, $s_1 = 1$ and $t_1 > r_1$ or if $\psi(1) = 1$, $r_1 = 1$ and $t_1 > s_1$, then*

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0.$$

(b) *If $t_1 < \min(r_1, s_1)$, then $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0$ for any $(\varphi, \psi) \in \mathfrak{I}_{k,\ell}$.*

Proof. (a). We only consider the case when $\varphi(1) = 1$, $s_1 = 1$ and $t_1 > r_1$. The proof of the other case is similar. Since $\varphi(1) = 1$, we have $\psi(1) > 1$. This means that $h_{(\varphi,\psi),i} = r_i$ for $1 \leqslant i \leqslant \psi(1) - 1$ and $h_{(\varphi,\psi),\psi(1)} = s_1$. Suppose $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \neq 0$. Then by Lemma 3.1, we have $t_i \geqslant r_i$ for $2 \leqslant i \leqslant \psi(1) - 1$ and $\sum\limits_{j=1}^{\psi(1)-1} r_j + s_1 > \sum\limits_{j=1}^{\psi(1)-1} t_j$ by taking $i = \psi(1)$. From these two inequalities, we obtain $r_1 + s_1 > t_1$ and hence $r_1 \geqslant t_1$ since $s_1 = 1$. This is a contradiction.
(b) If $t_1 < \min(r_1, s_1)$, then $t_1 < h_{(\varphi,\psi),1}$. So by Lemma 3.1, for every $(\varphi, \psi) \in \mathfrak{I}_{k,\ell}$ we have $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0$. □

We next give some relations among the numbers $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)$ as the parameters vary.

Definition 3.3. *Let* $\vec{e}_1$ *denote* $(1, 0, \cdots, 0)$ *of suitable dimension. So for any vector* $\vec{x} = (x_1, x_2, \cdots, x_k)$ *and* $a \in \mathbb{Z}$*, we have*

$$\vec{x} - a\vec{e}_1 = (x_1 - a, x_2, \cdots, x_k).$$

Define

$$\vec{x}\,' = (x'_1, \cdots, x'_{k-1}) := (x_2, \cdots, x_k)$$

with the convention that $(x_1)' = \mathbf{e}$*. For a function* f *on* $[k]$*, let* $f^\sharp$ *and* $f^\flat$ *be respectively the functions on* $[k-1]$ *and* $[k]$ *defined by*

$$f^\sharp(x) = f(x+1) - 1, \quad f^\flat(x) = f(x) - 1$$

with the convention that $[0] = \emptyset$ *and that, if* f *is a function on* $[1]$*, then* $f^\sharp = \mathbf{f}$*. Let* $f^\&$ *and* f^* *be respectively the functions on* $[k+1]$ *and* $[k]$ *defined by*

$$f^\&(1) = 1, \; f^\&(x) = f(x-1) + 1, \quad f^*(y) = f(y) + 1, \quad 2 \leqslant x \leqslant r+1, 1 \leqslant y \leqslant r.$$

Also define

$$\mathfrak{I}_{k,\ell,\varphi(1)=1} = \{(\varphi, \psi) \in \mathfrak{I}_{k,\ell} \mid \varphi(1) = 1\}, \quad \mathfrak{I}_{k,\ell,\psi(1)=1} = \{(\varphi, \psi) \in \mathfrak{I}_{k,\ell} \mid \psi(1) = 1\}.$$

Lemma 3.4. *Let* $k, \ell \geqslant 1$*. The map*

$$({}^\sharp, {}^\flat) : \mathfrak{I}_{k,\ell,\varphi(1)=1} \to \mathfrak{I}_{k-1,\ell}, \quad (\varphi, \psi) \mapsto (\varphi^\sharp, \psi^\flat)$$

is a bijection whose inverse is given by

$$({}^\&, {}^*) : \mathfrak{I}_{k-1,\ell} \to \mathfrak{I}_{k,\ell,\varphi(1)=1}, \quad (\varphi, \psi) \mapsto (\varphi^\&, \psi^*).$$

Similarly, the map

$$({}^\flat, {}^\sharp) : \mathfrak{I}_{k,\ell,\psi(1)=1} \to \mathfrak{I}_{k,\ell-1}, \quad (\varphi, \psi) \mapsto (\varphi^\flat, \psi^\sharp)$$

is a bijection whose inverse is given by

$$({}^*, {}^\&) : \mathfrak{I}_{k,\ell-1} \to \mathfrak{I}_{k,\ell,\psi(1)=1}, \quad (\varphi, \psi) \mapsto (\varphi^*, \psi^\&).$$

Proof. From the definition we verify that

$$({}^\sharp, {}^\flat)(\mathfrak{I}_{k,\ell,\varphi(1)=1}) \subseteq \mathfrak{I}_{k-1,\ell}$$

and

$$({}^\&, {}^*)(\mathfrak{I}_{k-1,\ell}) \subseteq \mathfrak{I}_{k,\ell,\varphi(1)=1}.$$

Then to prove the first assertion we only need to show that $(\varphi^\sharp)^\& = \varphi$ and $(\psi^\flat)^* = \psi$ if $\varphi(1) = 1$, and that $(\varphi^\&)^\sharp = \varphi$ and $(\psi^*)^\flat = \psi$. We just check the first equation and leave the others to the interested reader. First we have $(\varphi^\sharp)^\&(1) = 1$ by definition. Since $\varphi(1) = 1$, we have $(\varphi^\sharp)^\&(i) = \varphi(i)$ when $i = 1$. If $i \geqslant 2$, then by definition we have $\varphi^\sharp(i-1) = \varphi(i)-1$ and $(\varphi^\sharp)^\&(i) = \varphi^\sharp(i-1)+1 = \varphi(i)$, as desired.

The proof of the second assertion in the lemma is similar. □

Lemma 3.5. *Let* $k, \ell, \vec{r}, \vec{s}, \vec{t}$ *and* (φ, ψ) *be as in Lemma 3.1.*

(a) *Let a and b be integers such that $a < \min(t_1, r_1)$, $b < \min(t_1, s_1)$. Then for all $i \in \{2, \cdots, k+\ell\}$, we have*

$$c_{\vec{r}-a\vec{e}_1,\vec{s}}^{\vec{t}-a\vec{e}_1,(\varphi,\psi)}(i) = c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i)$$

and

$$c_{\vec{r},\vec{s}-b\vec{e}_1}^{\vec{t}-b\vec{e}_1,(\varphi,\psi)}(i) = c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i).$$

(b) *If $\varphi(1) = 1$ and $r_1 = t_1 = 1$, then*

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i+1) = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}(i), \quad 1 \leqslant i \leqslant k+\ell-1, \tag{36}$$

with the notations in Definition 3.3. Similarly, if $\psi(1) = 1$ and $s_1 = t_1 = 1$, then

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i+1) = c_{\vec{r},\vec{s}\,'}^{\vec{t}\,',(\varphi^\flat,\psi^\sharp)}(i), \quad 1 \leqslant i \leqslant k+\ell-1. \tag{37}$$

Proof. (a) We prove the first equality. The proof for the second equality is similar. Since $a < \min(r_1, t_1)$, we have $\vec{r} - a\vec{e}_1 \in \mathbb{Z}_{\geqslant 1}^k$ and $\vec{t} - a\vec{e}_1 \in \mathbb{Z}_{\geqslant 1}^{k+\ell}$. For better distinction, we will use the full notation $h_{(\varphi,\psi),(\vec{r},\vec{s}),i}$ defined in Eq. (31) instead of its abbreviation $h_{(\varphi,\psi),i}$. Then we have

$$h_{(\varphi,\psi),(\vec{r}-a\vec{e}_1,\vec{s}),i} = \begin{cases} h_{(\varphi,\psi),(\vec{r},\vec{s}),i} & \text{if } i \neq \varphi(1), \\ h_{(\varphi,\psi),(\vec{r},\vec{s}),i} - a & \text{if } i = \varphi(1). \end{cases} \tag{38}$$

Let $i \in \{2, \cdots, k+\ell\}$. If $\varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = 1$, then $i \neq \varphi(1)$. Indeed, if $i = \varphi(1)$, then $i-1$ must be in $\operatorname{im}(\psi)$, implying that $\varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = -1$. Thus

$$c_{\vec{r}-a\vec{e}_1,\vec{s}}^{\vec{t}-a\vec{e}_1,(\varphi,\psi)}(i) = \binom{t_i-1}{h_{(\varphi,\psi),(\vec{r}-a\vec{e}_1,\vec{s}),i}-1} = \binom{t_i-1}{h_{(\varphi,\psi),(\vec{r},\vec{s}),i}-1} = c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i).$$

If $\varepsilon_{\varphi,\psi}(i)\varepsilon_{\varphi,\psi}(i-1) = -1$, then either $i = \varphi(j)$ or $i-1 = \varphi(j)$ for some $j \in [k]$. In either case, we have $i \geqslant \varphi(1)$ since φ keeps the order. Thus by Eq. (38), we have

$$\sum_{j=1}^{i} h_{(\varphi,\psi),(\vec{r}-a\vec{e}_1,\vec{s}),j} = \sum_{j=1}^{i} h_{(\varphi,\psi),(\vec{r},\vec{s}),j} - a.$$

So

$$c_{\vec{r}-a\vec{e}_1,\vec{s}}^{\vec{t}-a\vec{e}_1,(\varphi,\psi)}(i) = \binom{t_i-1}{(t_1-a)+\sum\limits_{j=2}^{i} t_j - \sum\limits_{j=1}^{i} h_{(\varphi,\psi),(\vec{r}-a\vec{e}_1,\vec{s}),j}} = \binom{t_i-1}{\sum\limits_{j=1}^{i} t_j - \sum\limits_{j=1}^{i} h_{(\varphi,\psi),(\vec{r},\vec{s}),j}} = c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i).$$

(b) Let $\varphi(1) = 1$ and $r_1 = t_1 = 1$. By Eq. (31), for $1 \leqslant i \leqslant k+\ell-1$,

$$\begin{aligned} h_{(\varphi,\psi),(\vec{r},\vec{s}),i+1} &= \begin{cases} r_j & \text{if } i+1 = \varphi(j) \\ s_j & \text{if } i+1 = \psi(j) \end{cases} = \begin{cases} r'_{j-1} & \text{if } i = \varphi(j)-1 \\ s_j & \text{if } i = \psi(j)-1 \end{cases} \\ &= \begin{cases} r'_j & \text{if } i = \varphi(j+1)-1 \\ s_j & \text{if } i = \psi(j)-1 \end{cases} = \begin{cases} r'_j & \text{if } i = \varphi^\sharp(j) \\ s_j & \text{if } i = \psi^\flat(j). \end{cases} \end{aligned}$$

Thus

$$h_{(\varphi,\psi),(\vec{r},\vec{s}),i+1} = h_{(\varphi^\sharp,\psi^\flat),(\vec{r}\,',\vec{s}),i}, \; 1 \leqslant i \leqslant k+\ell-1. \tag{39}$$

Also, for $1 \leqslant i \leqslant k+\ell-1$, since $\varphi(1) = 1$, we have

$$i+1 \in \operatorname{im}(\varphi) \Leftrightarrow i+1 = \varphi(j),\, j \in \{2, \cdots, k\} \Leftrightarrow i = \varphi^\sharp(j-1),\, j-1 \in [k-1] \Leftrightarrow i \in \operatorname{im}(\varphi^\sharp).$$

Similarly, $i+1 \in \mathrm{im}(\psi) \Leftrightarrow i \in \mathrm{im}(\psi^\flat)$. Thus

$$\varepsilon_{\varphi,\psi}(i+1) = \varepsilon_{\varphi^\sharp,\psi^\flat}(i), 1 \leqslant i \leqslant k+\ell-1. \tag{40}$$

We now verify Eq. (36) for $i=1$. Since $\varphi(1)=1$, either $2=\varphi(2)$ or $2=\psi(1)$. If $2=\varphi(2)$, then $\varepsilon_{\varphi,\psi}(2)\varepsilon_{\varphi,\psi}(1)=1$ and so

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(2) = \binom{t_2-1}{r_2-1} = \binom{t'_1-1}{r'_1-1} = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}(1).$$

If $\psi(1)=2$, then $\varepsilon_{\varphi,\psi}(2)\varepsilon_{\varphi,\psi}(1)=-1$. So by the condition that $r_1=t_1=1$, we obtain

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(2) = \binom{t_2-1}{t_1+t_2-r_1-s_1} = \binom{t_2-1}{t_2-s_1} = \binom{t_2-1}{s_1-1} = \binom{t'_1-1}{s_1-1} = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}(1).$$

Next consider $i \geqslant 2$. By Eq. (39) and Eq. (40), we have

$$\begin{aligned} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i+1) &= \begin{cases} \dbinom{t_{i+1}-1}{h_{(\varphi,\psi),(\vec{r},\vec{s}),i+1}-1} & \text{if } \varepsilon_{\varphi,\psi}(i+1)\varepsilon_{\varphi,\psi}(i)=1, \\ \dbinom{t_{i+1}-1}{\sum_{j=1}^{i+1} t_j - \sum_{j=1}^{i+1} h_{(\varphi,\psi),(\vec{r},\vec{s}),j}} & \text{if } \varepsilon_{\varphi,\psi}(i+1)\varepsilon_{\varphi,\psi}(i)=-1, \end{cases} \\ &= \begin{cases} \dbinom{t'_i-1}{h_{(\varphi^\sharp,\psi^\flat),(\vec{r}\,',\vec{s}),i}-1} & \text{if } \varepsilon_{\varphi^\sharp,\psi^\flat}(i)\varepsilon_{\varphi^\sharp,\psi^\flat}(i-1)=1, \\ \dbinom{t'_i-1}{\sum_{j=1}^{i} t'_j - \sum_{j=1}^{i} h_{(\varphi^\sharp,\psi^\flat),(\vec{r}\,',\vec{s}),j}} & \text{if } \varepsilon_{\varphi^\sharp,\psi^\flat}(i)\varepsilon_{\varphi^\sharp,\psi^\flat}(i-1)=-1, \end{cases} \end{aligned}$$

since $t_1=1$ and $h_{(\varphi,\psi),(\vec{r},\vec{s}),1}=r_1=1$. Therefore, we have $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i+1) = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}(i)$ when $i \geqslant 2$.

The proof for Eq. (37) is similar. □

Lemma 3.6. *Let $k,\ell,\vec{r},\vec{s},\vec{t}$ and (φ,ψ) be as in Lemma 3.1.*

(a) *Suppose that $r_1 \geqslant 2$ and $s_1 \geqslant 2$. If $t_1 \geqslant 2$, then we have*

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = c_{\vec{r}-\vec{e}_1,\vec{s}}^{\vec{t}-\vec{e}_1,(\varphi,\psi)} + c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)} \tag{41}$$

If $t_1=1$, then we have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0. \tag{42}$$

(b) *Suppose that $r_1=s_1=1$. If $\varphi(1)=1$ and $t_1=1$, then we have*

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)} \tag{43}$$

with the notations in Definition 3.3. If $\psi(1)=1$ and $t_1=1$, then we have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = c_{\vec{r},\vec{s}\,'}^{\vec{t}\,',(\varphi^\flat,\psi^\sharp)}. \tag{44}$$

If $t_1 \geqslant 2$, then we have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0. \tag{45}$$

(c) *Suppose that* $r_1 = 1$ *and* $s_1 \geqslant 2$. *If* $\varphi(1) = 1$ *and* $t_1 = 1$, *then we have*

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = c^{\vec{t}',(\varphi^\sharp,\psi^\flat)}_{\vec{r}',\vec{s}}. \tag{46}$$

If $\psi(1) = 1$ *and* $t_1 = 1$, *then we have*

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = 0. \tag{47}$$

If $t_2 \geqslant 2$, *then we have*

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}. \tag{48}$$

Similar statements hold when $r_1 \geqslant 2$ *and* $s_1 = 1$.

Proof. (a) If $\varphi(1) = 1$, then

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(1) = \binom{t_1-1}{r_1-1} = \binom{t_1-2}{r_1-2} + \binom{t_1-2}{r_1-1} = c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r}-\vec{e}_1,\vec{s}}(1) + c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}(1).$$

Similarly, if $\psi(1) = 1$, we also have

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(1) = c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r}-\vec{e}_1,\vec{s}}(1) + c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}(1).$$

In either case, by Lemma 3.5.(a) we have

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i) = c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r}-\vec{e}_1,\vec{s}}(i) = c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}(i)$$

when $i \in \{2, \cdots, k+\ell\}$. Hence

$$\begin{aligned}
c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} &= \prod_{i=1}^{k+\ell} c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i) \\
&= \left(c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r}-\vec{e}_1,\vec{s}}(1) + c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}(1)\right) \prod_{i=2}^{k+\ell} c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i) \\
&= \prod_{i=1}^{k+\ell} c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r}-\vec{e}_1,\vec{s}}(i) + \prod_{i=1}^{k+\ell} c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}(i) \\
&= c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r}-\vec{e}_1,\vec{s}} + c^{\vec{t}-\vec{e}_1,(\varphi,\psi)}_{\vec{r},\vec{s}-\vec{e}_1}.
\end{aligned}$$

This proves Eq. (41). Eq (42) follows from Lemma 3.2 (b).

(b) First we assume that $t_1 = 1$. For $(\varphi, \psi) \in \mathfrak{I}_{k,\ell}$, either $\varphi(1) = 1$ or $\psi(1) = 1$. If $\varphi(1) = 1$, then

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(1) = \binom{t_1-1}{r_1-1} = \binom{0}{0} = 1$$

and by Lemma 3.5.(b) we have

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i+1) = c^{\vec{t}',(\varphi^\sharp,\psi^\flat)}_{\vec{r}',\vec{s}}(i).$$

Hence

$$c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}} = \prod_{i=1}^{k+\ell} c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i) = \prod_{i=2}^{k+\ell} c^{\vec{t},(\varphi,\psi)}_{\vec{r},\vec{s}}(i) = \prod_{i=1}^{k+\ell-1} c^{\vec{t}',(\varphi^\sharp,\psi^\flat)}_{\vec{r}',\vec{s}}(i) = c^{\vec{t}',(\varphi^\sharp,\psi^\flat)}_{\vec{r}',\vec{s}}.$$

This proves Eq. (43). The proof of Eq. (44) is similar. The equality for $t_1 \geqslant 2$ follows from Lemma 3.2.(a).

(c) Suppose that $r_1 = 1$ and $s_1 \geqslant 2$.

Case 1: $t_1 = 1$**.** We consider the case of $\varphi(1) = 1$. By Lemma 3.5.(b) we have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i+1) = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}(i).$$

Combining this with

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(1) = \binom{t_1-1}{r_1-1} = \binom{0}{0} = 1,$$

we obtain

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = \prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) = \prod_{i=1}^{k+\ell-1} c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}(i) = c_{\vec{r}\,',\vec{s}}^{\vec{t}\,',(\varphi^\sharp,\psi^\flat)}.$$

This proves Eq. (46). If $\psi(1) = 1$, then

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(1) = \binom{t_1-1}{s_1-1} = \binom{0}{s_1-1} = 0$$

since $s_1 - 1 \geqslant 1$ and so $c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0$, as needed.

Case 2: $t_1 \geqslant 2$**.** We will consider the four subcases when $\psi(1) = 1$ and $t_1 < s_1$, when $\psi(1) = 1$ and $t_1 > s_1$, when $\psi(1) = 1$ and $t_1 = s_1$, and when $\varphi(1) = 1$.

If $\psi(1) = 1$ and $t_1 < s_1$, then

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0 = c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}$$

by Lemma 3.1. If $\psi(1) = 1$ and $t_1 > s_1$, then by Lemma 3.2.(a) we also have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = 0 = c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}.$$

So in these two subcases (48) holds.

Now if $\psi(1) = 1$ and $t_1 = s_1$, then

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(1) = \binom{t_1-1}{s_1-1} = 1 = \binom{t_1-2}{s_1-2} = c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}(1).$$

If $\varphi(1) = 1$, then since $r_1 = 1$, we have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(1) = \binom{t_1-1}{r_1-1} = \binom{t_1-1}{0} = 1 = \binom{t_1-2}{0} = \binom{t_1-2}{r_1-1} = c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}(1).$$

In both subcases, by Lemma 3.5.(a) we always have

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) = c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}(i).$$

for $i \geqslant 2$. Therefore,

$$c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} = \prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)}(i) = \prod_{i=1}^{k+\ell} c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}(i) = c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}.$$

This proves (48).

The proof for the instance of $r_1 \geqslant 2$ and $s_1 = 1$ is similar. □

4. Proof of the main theorems

We first show that, under the condition that G is an abelian group, Theorem 2.1 and Theorem 2.2 are equivalent. Then we only need to prove Theorem 2.1. This is done in Section 4.2.

4.1. **The equivalence between Theorem 2.1 and Theorem 2.2.** We start with a lemma.

Lemma 4.1. *Let G be an abelian group. With the notations in Eq. (12), (17) and (22), we have*

$$\theta(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b}) = \theta(\vec{a}) \star_{(\varphi,\psi)} \theta(\vec{b}). \tag{49}$$

Proof. Let $\vec{w} = \theta(\vec{a})$ and $\vec{z} = \theta(\vec{b})$. Then by Eq. (12), we have $w_j = 1/a_1$ when $j = 1$ and $w_j = a_{j-1}/a_j$ when $j \geqslant 2$. Similarly, $z_j = 1/b_1$ when $j = 1$ and $z_j = b_{j-1}/b_j$ when $j \geqslant 2$.

Recall Eq. (17):

$$(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_i = \begin{cases} a_j & \text{if } i = \varphi(j), \\ b_j & \text{if } i = \psi(j). \end{cases}$$

When $i = 1$, we have

$$\theta(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_1 = (\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_1^{-1} = \begin{cases} a_1^{-1} = w_1 & \text{if } 1 = \varphi(1) \\ b_1^{-1} = z_1 & \text{if } 1 = \psi(1) \end{cases} = (\vec{w} \star_{(\varphi,\psi)} \vec{z})_1.$$

Next let $i \geqslant 2$. Assume that $i \in \mathrm{im}(\varphi)$, say $i = \varphi(j)$ for some $j \in [k]$. If $i - 1 \in \mathrm{im}(\varphi)$, then $j \geqslant 2$ and $i - 1 = \varphi(j - 1)$. Thus

$$\theta(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_i = \frac{(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_{i-1}}{(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_i} = \frac{a_{j-1}}{a_j} = w_j.$$

If $i - 1 \in \mathrm{im}(\psi)$, then $i - 1 = \psi(i - j)$. Thus

$$\theta(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_i = \frac{(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_{i-1}}{(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_i} = \frac{b_{i-j}}{a_j} = \frac{(z_1 \cdots z_{i-j})^{-1}}{(w_1 \cdots w_j)^{-1}} = \frac{w_1 \cdots w_j}{z_1 \cdots z_{i-j}}.$$

Hence by Eq. (22),

$$\theta(\vec{a} \sqcup\!\sqcup_{(\varphi,\psi)} \vec{b})_i = (\vec{w} \star_{(\varphi,\psi)} \vec{z})_i$$

when $i \in \mathrm{im}(\varphi)$. A similar argument shows that the above equality also holds when $i \in \mathrm{im}(\psi)$. This proves (49). $\square$

Proposition 4.2. *When G is an abelian group, Theorem 2.2 is equivalent to Theorem 2.1.*

Proof. From the definitions of θ, $\shuffle_\eta$ and $\shuffle_\rho$, we see that θ is an algebra isomorphism from $\mathcal{H}^{\shuffle_\rho}(\widehat{G}) = (\mathcal{H}(\widehat{G}), \shuffle_\rho)$ to $\mathcal{H}^{\shuffle_\eta}(\widehat{G}) = (\mathcal{H}(\widehat{G}), \shuffle_\eta)$. So for any $\left[\begin{smallmatrix} \vec{r} \\ \vec{a} \end{smallmatrix}\right], \left[\begin{smallmatrix} \vec{s} \\ \vec{b} \end{smallmatrix}\right] \in \mathcal{H}^{\shuffle_\rho}(\widehat{G})$,

$$\begin{aligned}
& \left[\begin{smallmatrix} \vec{r} \\ \vec{a} \end{smallmatrix}\right] \shuffle_\rho \left[\begin{smallmatrix} \vec{s} \\ \vec{b} \end{smallmatrix}\right] = \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell} \\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell}, |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \left[\begin{smallmatrix} \vec{t} \\ \vec{a} \shuffle_{(\varphi,\psi)} \vec{b} \end{smallmatrix}\right] \\
\Leftrightarrow\ & \theta\left(\left[\begin{smallmatrix} \vec{r} \\ \vec{a} \end{smallmatrix}\right] \shuffle_\rho \left[\begin{smallmatrix} \vec{s} \\ \vec{b} \end{smallmatrix}\right]\right) = \theta\Big(\sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell} \\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell}, |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \left[\begin{smallmatrix} \vec{t} \\ \vec{a} \shuffle_{(\varphi,\psi)} \vec{b} \end{smallmatrix}\right]\Big) \\
\Leftrightarrow\ & \theta\left(\left[\begin{smallmatrix} \vec{r} \\ \vec{a} \end{smallmatrix}\right]\right) \shuffle_\eta \theta\left(\left[\begin{smallmatrix} \vec{s} \\ \vec{b} \end{smallmatrix}\right]\right) = \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell} \\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell}, |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \theta\left(\left[\begin{smallmatrix} \vec{t} \\ \vec{a} \shuffle_{(\varphi,\psi)} \vec{b} \end{smallmatrix}\right]\right) \\
\Leftrightarrow\ & \left[\begin{smallmatrix} \vec{r} \\ \theta(\vec{a}) \end{smallmatrix}\right] \shuffle_\eta \left[\begin{smallmatrix} \vec{s} \\ \theta(\vec{b}) \end{smallmatrix}\right] = \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell} \\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell}, |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \left[\begin{smallmatrix} \vec{t} \\ \theta(\vec{a} \shuffle_{(\varphi,\psi)} \vec{b}) \end{smallmatrix}\right] \\
\Leftrightarrow\ & \left[\begin{smallmatrix} \vec{r} \\ \theta(\vec{a}) \end{smallmatrix}\right] \shuffle_\eta \left[\begin{smallmatrix} \vec{s} \\ \theta(\vec{b}) \end{smallmatrix}\right] = \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell} \\ \vec{t}\in\mathbb{Z}_{\geqslant 1}^{k+\ell}, |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \left[\begin{smallmatrix} \vec{t} \\ \theta(\vec{a}) \star_{(\varphi,\psi)} \theta(\vec{b}) \end{smallmatrix}\right] \qquad \text{(by Eq. (49)).}
\end{aligned}$$

Then the proposition follows from the bijectivity of θ. □

4.2. **Proof of Theorem 2.1.** In this section we prove Theorem 2.1. We first describe recursive relations of $\shuffle_\rho$ that we will use later in the proof.

Let $\mathcal{H}^{\shuffle_\rho +}(\widehat{G})$ be the subring of $\mathcal{H}^{\shuffle_\rho}(\widehat{G})$ generated by $\left[\begin{smallmatrix} \vec{s} \\ \vec{b} \end{smallmatrix}\right]$ with $\vec{s} \in \mathbb{Z}_{\geqslant 1}^k, \vec{b} \in G^k, k \geqslant 1$. Then

$$\mathcal{H}^{\shuffle_\rho}(\widehat{G}) = \mathbb{Z} \oplus \mathcal{H}^{\shuffle_\rho +}(\widehat{G}).$$

Define the following operators

$$P : \mathcal{H}^{\shuffle_\rho +}(\widehat{G}) \to \mathcal{H}^{\shuffle_\rho}(\widehat{G}), \quad P\left(\left[\begin{smallmatrix} s_1, s_2, \cdots, s_k \\ b_1, b_2, \cdots, b_k \end{smallmatrix}\right]\right) = \left[\begin{smallmatrix} s_1+1, s_2, \cdots, s_k \\ b_1, b_2, \cdots, b_k \end{smallmatrix}\right],$$

$$Q_b : \mathcal{H}^{\shuffle_\rho}(\widehat{G}) \to \mathcal{H}^{\shuffle_\rho}(\widehat{G}), \quad Q_b\left(\left[\begin{smallmatrix} s_1, \cdots, s_k \\ b_1, \cdots, b_k \end{smallmatrix}\right]\right) = \left[\begin{smallmatrix} 1, s_1, \cdots, s_k \\ b, b_1, \cdots, b_k \end{smallmatrix}\right], \quad Q_b(1) = \left[\begin{smallmatrix} 1 \\ b \end{smallmatrix}\right].$$

Proposition 4.3. *The multiplication $\shuffle_\rho$ on $\mathcal{H}^{\shuffle_\rho}(\widehat{G})$ defined in Eq. (14) is the unique one that satisfies the Rota-Baxter type relations* [18]*:*

$$\begin{aligned}
& P(\xi_1) \shuffle_\rho P(\xi_2) = P(\xi_1 \shuffle_\rho P(\xi_2)) + P(P(\xi_1) \shuffle_\rho \xi_2),\ \xi_1, \xi_2 \in \mathcal{H}^{\shuffle_\rho +}(\widehat{G}), \\
& Q_a(\xi_1) \shuffle_\rho Q_b(\xi_2) = Q_a(\xi_1 \shuffle_\rho Q_b(\xi_2)) + Q_b(Q_a(\xi_1) \shuffle_\rho \xi_2),\ \xi_1, \xi_2 \in \mathcal{H}^{\shuffle_\rho}(\widehat{G}), \\
& P(\xi_1) \shuffle_\rho Q_b(\xi_2) = Q_b(P(\xi_1) \shuffle_\rho \xi_2) + P(\xi_1 \shuffle_\rho Q_b(\xi_2)),\ \xi_1 \in \mathcal{H}^{\shuffle_\rho +}(\widehat{G}), \xi_2 \in \mathcal{H}^{\shuffle_\rho}(\widehat{G}), \\
& Q_b(\xi_1) \shuffle_\rho P(\xi_2) = Q_b(\xi_1 \shuffle_\rho P(\xi_2)) + P(Q_b(\xi_1) \shuffle_\rho \xi_2),\ \xi_1 \in \mathcal{H}^{\shuffle_\rho}(\widehat{G}), \xi_2 \in \mathcal{H}^{\shuffle_\rho +}(\widehat{G}).
\end{aligned}$$

with the initial condition that $1 \shuffle_\rho \xi = \xi \shuffle_\rho 1 = \xi$ *for* $\xi \in \mathcal{H}^{\shuffle_\rho}(\widehat{G})$.

Proof. Let $\mathcal{H}_1^{ш+}(\overline{G})$ be the subring of $\mathcal{H}_1^{ш}(\overline{G})$ generated by words of the form ux_b with $b \in G$. Then

$$\mathcal{H}_1^{ш}(\overline{G}) = \mathbb{Z} \oplus \mathcal{H}_1^{ш+}(\overline{G}).$$

Define operators

$$I_0 : \mathcal{H}_1^{ш+}(\overline{G}) \to \mathcal{H}_1^{ш}(\overline{G}), \quad I_0(u) = x_0 u,$$

$$I_b : \mathcal{H}_1^{ш}(\overline{G}) \to \mathcal{H}_1^{ш}(\overline{G}), \quad I_b(u) = \begin{cases} x_b u, & u \neq 1, \\ x_b, & u = 1, \end{cases}$$

for $b \in G$. Then the well-known recursive formula of the shuffle product

$$(a_1\mathfrak{a}) ш (b_1\mathfrak{b}) = a_1(\mathfrak{a} ш (b_1\mathfrak{b})) + b_1((a_1\mathfrak{a}) ш \mathfrak{b}), a_1, b_1 \in \overline{G}, \mathfrak{a}, \mathfrak{b} \in M(\overline{G})$$

can be rewritten as the following relations of I_0 and I_a, I_b, $a, b \in G$,

$$\begin{aligned} I_0(u) ш I_0(v) &= I_0(u ш I_0(v)) + I_0(I_0(u) ш v), \quad u, v \in \mathcal{H}_1^{ш+}(\overline{G}), \\ I_a(u) ш I_b(v) &= I_a(u ш I_b(v)) + I_b(I_a(u) ш v), \quad u, v \in \mathcal{H}_1^{ш}(\overline{G}), \\ I_0(u) ш I_b(v) &= I_0(u ш I_b(v)) + I_b(I_0(u) ш v), \quad u \in \mathcal{H}_1^{ш+}(\overline{G}), v \in \mathcal{H}_1^{ш}(\overline{G}), \\ I_b(u) ш I_0(v) &= I_b(u ш I_0(v)) + I_0(I_b(u) ш v), \quad u \in \mathcal{H}_1^{ш}(\overline{G}), v \in \mathcal{H}_1^{ш+}(\overline{G}). \end{aligned} \tag{50}$$

Under the bijection $\rho : \mathcal{H}_1^{ш}(\overline{G}) \to \mathcal{H}^{ш_\rho}(\widehat{G})$ in Eq. (13), I_0 and I_b, $b \in G$, are sent to P and Q_b, $b \in G$, respectively. Further the relations in Eq. (50) for I_0 and I_b, $b \in G$, take the form in Proposition 4.3. Finally, since $ш$ is the unique multiplication on $\mathcal{H}_1^{ш}(\overline{G})$ characterized by its recursive relation Eq. (50) and the initial condition $1 ш u = u ш 1 = u$, $ш_\rho$ is also unique as characterized. ◻

For $\vec{b} \in G^k$, recall the following notation from Definition 3.3:

$$\vec{b}\,' = (b_1', \cdots, b_{k-1}') := (b_2, \cdots, b_k)$$

with the convention that $\vec{b}\,' = \mathbf{e}$ when $k = 1$. In the proof for Theorem 2.1 we also need the following lemma.

Lemma 4.4. *Let $\vec{t} \in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}$, $\vec{a} \in G^k$ and $\vec{b} \in G^\ell$.*

(a) *For any $(\varphi, \psi) \in \mathfrak{I}_{k-1,\ell}$ we have*

$$Q_{a_1}\left(\left[\begin{smallmatrix} \vec{t} \\ \vec{a}\,' ш_{(\varphi,\psi)} \vec{b} \end{smallmatrix}\right]\right) = \left[\begin{smallmatrix} (1,\vec{t}) \\ \vec{a} ш_{(\varphi^{\&},\psi^*)} \vec{b} \end{smallmatrix}\right] \tag{51}$$

with the notations in Eq. (17) and Definition 3.3.

(b) *For any $(\varphi, \psi) \in \mathfrak{I}_{k,\ell-1}$ we have*

$$Q_{b_1}\left(\left[\begin{smallmatrix} \vec{t} \\ \vec{a} ш_{(\varphi,\psi)} \vec{b}\,' \end{smallmatrix}\right]\right) = \left[\begin{smallmatrix} (1,\vec{t}) \\ \vec{a} ш_{(\varphi^*,\psi^{\&})} \vec{b} \end{smallmatrix}\right]. \tag{52}$$

Proof. (a) Let $\vec{\varpi} = (\varpi_1, \cdots, \varpi_{k+\ell-1}) := \vec{a}\,' ш_{(\varphi,\psi)} \vec{b}$ and $\vec{\tau} = (\tau_1, \cdots, \tau_{k+\ell}) := \vec{a} ш_{(\varphi^{\&},\psi^*)} \vec{b}$. By the definition of Q_{a_1}, we only need to prove that

$$\tau_i = \begin{cases} a_1 & \text{if } i = 1, \\ \varpi_{i-1} & \text{if } i \geqslant 2. \end{cases}$$

Since $\varphi^{\&}(1) = 1$, we have $\tau_1 = a_1$. Now let $i \geqslant 2$. We have $i \in \mathrm{im}(\varphi^{\&})$ or $i \in \mathrm{im}(\psi^*)$. If $i \in \mathrm{im}(\varphi^{\&})$, say $i = \varphi^{\&}(j)$, then $i - 1 = \varphi(j - 1)$. Thus we have $\tau_i = a_j$ and $\varpi_{i-1} = a'_{j-1} = a_j$. This shows that $\tau_i = \varpi_{i-1}$. If $i \in \mathrm{im}(\psi^*)$, say $i = \psi^*(j)$, then $i - 1 = \psi(j)$. Thus $\tau_i = b_j$ and $\varpi_{i-1} = b_j$ again showing $\tau_i = \varpi_{i-1}$.

(b). The proof is similar to that for Item. (a). $\square$

Proof of Theorem 2.1. We prove the extended form of (21) where one of k and ℓ, but not both, might be zero. We prove this by induction on $|\vec{r}| + |\vec{s}| \geqslant 1$. If $|\vec{r}| + |\vec{s}| = 1$, then exactly one of k and ℓ is zero. So exactly one of $\begin{bmatrix} \vec{r} \\ \vec{a} \end{bmatrix}$ and $\begin{bmatrix} \vec{s} \\ \vec{b} \end{bmatrix}$ is the identity 1. Then by (34) and (35), there is nothing to prove. For any given integer $n \geqslant 2$, assume that the assertion holds for every pair $(\vec{r}, \vec{s})$ with $|\vec{r}| + |\vec{s}| < n$. Now consider $\vec{r}$ and $\vec{s}$ with $|\vec{r}| + |\vec{s}| = n$. If one of k or ℓ is 0, then again by (34) and (35) there is nothing to prove. So we may assume that $k, \ell \geqslant 1$. There are four cases to consider.

Case 1. $r_1 \geqslant 2$ **and** $s_1 \geqslant 2$**.** Then by Proposition 4.3 and the induction hypothesis, we have

$$
\begin{aligned}
\begin{bmatrix} \vec{r} \\ \vec{a} \end{bmatrix} Ш_\rho \begin{bmatrix} \vec{s} \\ \vec{b} \end{bmatrix}
&= P\left(\begin{bmatrix} \vec{r}-\vec{e}_1 \\ \vec{a} \end{bmatrix}\right) Ш_\rho P\left(\begin{bmatrix} \vec{s}-\vec{e}_1 \\ \vec{b} \end{bmatrix}\right) \\
&= P\left(\begin{bmatrix} \vec{r}-\vec{e}_1 \\ \vec{a} \end{bmatrix} Ш_\rho \begin{bmatrix} \vec{s} \\ \vec{b} \end{bmatrix} + \begin{bmatrix} \vec{r} \\ \vec{a} \end{bmatrix} Ш_\rho \begin{bmatrix} \vec{s}-\vec{e}_1 \\ \vec{b} \end{bmatrix}\right) \\
&= P\Bigg(\sum_{(\varphi,\psi)\in \mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} \left(c_{\vec{r}-\vec{e}_1,\vec{s}}^{\vec{t},(\varphi,\psi)} + c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t},(\varphi,\psi)}\right) \begin{bmatrix} \vec{t} \\ \vec{a}\, Ш_{(\varphi,\psi)} \vec{b} \end{bmatrix} \Bigg) \\
&= \sum_{(\varphi,\psi)\in \mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} \left(c_{\vec{r}-\vec{e}_1,\vec{s}}^{\vec{t},(\varphi,\psi)} + c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t},(\varphi,\psi)}\right) \begin{bmatrix} \vec{t}+\vec{e}_1 \\ \vec{a}\, Ш_{(\varphi,\psi)} \vec{b} \end{bmatrix} \\
&= \sum_{(\varphi,\psi)\in \mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|, t_1\geqslant 2}} \left(c_{\vec{r}-\vec{e}_1,\vec{s}}^{\vec{t}-\vec{e}_1,(\varphi,\psi)} + c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t}-\vec{e}_1,(\varphi,\psi)}\right) \begin{bmatrix} \vec{t} \\ \vec{a}\, Ш_{(\varphi,\psi)} \vec{b} \end{bmatrix} \\
&= \sum_{(\varphi,\psi)\in \mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|, t_1\geqslant 2}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t} \\ \vec{a}\, Ш_{(\varphi,\psi)} \vec{b} \end{bmatrix} \qquad \text{(by Eq. (41))} \\
&= \sum_{(\varphi,\psi)\in \mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t} \\ \vec{a}\, Ш_{(\varphi,\psi)} \vec{b} \end{bmatrix} \qquad \text{(by Eq. (42)).}
\end{aligned}
$$

Case 2. $r_1 = s_1 = 1$**.** We will use the notations $\vec{r}\,', \vec{s}\,', \vec{a}\,'$ and $\vec{b}\,'$ in Definitions 3.3. Then

$$
\begin{aligned}
\begin{bmatrix} \vec{r} \\ \vec{a} \end{bmatrix} Ш_\rho \begin{bmatrix} \vec{s} \\ \vec{b} \end{bmatrix} &= Q_{a_1}\left(\begin{bmatrix} \vec{r}\,' \\ \vec{a}\,' \end{bmatrix}\right) Ш_\rho Q_{b_1}\left(\begin{bmatrix} \vec{s}\,' \\ \vec{b}\,' \end{bmatrix}\right) \\
&= Q_{a_1}\left(\begin{bmatrix} \vec{r}\,' \\ \vec{a}\,' \end{bmatrix} Ш_\rho \begin{bmatrix} \vec{s} \\ \vec{b} \end{bmatrix}\right) + Q_{b_1}\left(\begin{bmatrix} \vec{r} \\ \vec{a} \end{bmatrix} Ш_\rho \begin{bmatrix} \vec{s}\,' \\ \vec{b}\,' \end{bmatrix}\right)
\end{aligned}
$$

$$\begin{aligned}
&= Q_{a_1}\Big(\sum_{(\varphi,\psi)\in\mathfrak{I}_{k-1,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r}\,',\vec{s}}^{\vec{t},(\varphi,\psi)} \Big[\begin{array}{c} \vec{t} \\ \vec{a}\,' \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big]\Big) \\
&\quad + Q_{b_1}\Big(\sum_{(\varphi,\psi)\in\mathfrak{I}_{k,\ell-1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}\,'}^{\vec{t},(\varphi,\psi)} \Big[\begin{array}{c} \vec{t} \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b}\,' \end{array} \Big]\Big) \\
&= \sum_{(\varphi,\psi)\in\mathfrak{I}_{k-1,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r}\,',\vec{s}}^{\vec{t},(\varphi,\psi)} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi^{\&},\psi^{*})} \vec{b} \end{array} \Big] \\
&\quad + \sum_{(\varphi,\psi)\in\mathfrak{I}_{k,\ell-1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}\,'}^{\vec{t},(\varphi,\psi)} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi^{*},\psi^{\&})} \vec{b} \end{array} \Big] \quad (\text{ by Eq.(51) and (52)}) \\
&= \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}\\ \varphi(1)=1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r}\,',\vec{s}}^{\vec{t},(\varphi^{\sharp},\psi^{\flat})} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \\
&\quad + \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}\\ \psi(1)=1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}\,'}^{\vec{t},(\varphi^{\flat},\psi^{\sharp})} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \quad (\text{by Lemma 3.4}) \\
&= \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}\\ \varphi(1)=1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{(1,\vec{t}),(\varphi,\psi)} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \\
&\quad + \sum_{\substack{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}\\ \psi(1)=1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{(1,\vec{t}),(\varphi,\psi)} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \quad (\text{by Eq. (43) and (44)}) \\
&= \sum_{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{(1,\vec{t}),(\varphi,\psi)} \Big[\begin{array}{c} (1,\vec{t}) \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \\
&= \sum_{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|, t_1=1}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \Big[\begin{array}{c} \vec{t} \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \\
&= \sum_{(\varphi,\psi)\in\mathfrak{I}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell}\\ |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \Big[\begin{array}{c} \vec{t} \\ \vec{a} \, ш_{(\varphi,\psi)} \vec{b} \end{array} \Big] \qquad (\text{by Eq. (45)}).
\end{aligned}$$

Case 3. $r_1 = 1$ **and** $s_1 \geqslant 2$**.** With the notations in Definitions 3.3, we write $\vec{r} = (1, \vec{r}\,')$. Let $\vec{a}\,' = (a_2, \cdots, a_r)$. Then

$$\Big[\begin{array}{c} \vec{r} \\ \vec{a} \end{array} \Big] ш_\rho \Big[\begin{array}{c} \vec{s} \\ \vec{b} \end{array} \Big] = Q_{a_1}\Big(\Big[\begin{array}{c} \vec{r}\,' \\ \vec{a}\,' \end{array} \Big]\Big) ш_\rho P\Big(\Big[\begin{array}{c} \vec{s}-\vec{e}_1 \\ \vec{b} \end{array} \Big]\Big)$$

$$
\begin{aligned}
&= Q_{a_1}\Big(\begin{bmatrix} \vec{r}\,' \\ \vec{a}\,' \end{bmatrix} \text{Ш}_\rho \begin{bmatrix} \vec{s} \\ \vec{b} \end{bmatrix}\Big) + P\Big(\begin{bmatrix} \vec{r} \\ \vec{a} \end{bmatrix} \text{Ш}_\rho \begin{bmatrix} \vec{s}-\vec{e}_1 \\ \vec{b} \end{bmatrix}\Big) \\
&= Q_{a_1}\Big(\sum_{(\varphi,\psi)\in\mathfrak{J}_{k-1,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r}\,',\vec{s}}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t} \\ \vec{a}\,' \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix}\Big) \\
&\qquad + P\Big(\sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t} \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix}\Big) \\
&= \sum_{(\varphi,\psi)\in\mathfrak{J}_{k-1,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r}\,',\vec{s}}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} (1,\vec{t}) \\ \vec{a} \,\text{Ш}_{(\varphi^{\&},\psi^{*})} \vec{b} \end{bmatrix} \\
&\qquad + \sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}-\vec{e}_1}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t}+\vec{e}_1 \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \quad \text{(by Eq. (51))} \\
&= \sum_{\substack{(\varphi,\psi)\in\mathfrak{J}_{k,\ell} \\ \varphi(1)=1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r}\,',\vec{s}}^{\vec{t},(\varphi^{\sharp},\psi^{\flat})} \begin{bmatrix} (1,\vec{t}) \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \\
&\qquad + \sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}\,'}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t}+\vec{e}_1 \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \quad \text{(by Lemma 3.4)} \\
&= \sum_{\substack{(\varphi,\psi)\in\mathfrak{J}_{k,\ell} \\ \varphi(1)=1}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{(1,\vec{t}),(\varphi,\psi)} \begin{bmatrix} (1,\vec{t}) \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \\
&\qquad + \sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{\vec{t}+\vec{e}_1,(\varphi,\psi)} \begin{bmatrix} \vec{t}+\vec{e}_1 \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \quad \text{(by Eq. (46) and (48))} \\
&= \sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell-1} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{(1,\vec{t}),(\varphi,\psi)} \begin{bmatrix} (1,\vec{t}) \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \\
&\qquad + \sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|-1}} c_{\vec{r},\vec{s}}^{\vec{t}+\vec{e}_1,(\varphi,\psi)} \begin{bmatrix} \vec{t}+\vec{e}_1 \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix} \quad \text{(by Eq. (47))} \\
&= \sum_{(\varphi,\psi)\in\mathfrak{J}_{k,\ell}} \sum_{\substack{\vec{t}\in \mathbb{Z}_{\geqslant 1}^{k+\ell} \\ |\vec{t}|=|\vec{r}|+|\vec{s}|}} c_{\vec{r},\vec{s}}^{\vec{t},(\varphi,\psi)} \begin{bmatrix} \vec{t} \\ \vec{a} \,\text{Ш}_{(\varphi,\psi)} \vec{b} \end{bmatrix}.
\end{aligned}
$$

Case 4. $r_1 \geqslant 2$ **and** $s_1 = 1$**.** The proof for this case is similar to that for Case 3. $\square$

5. Appendix: a shuffle formulation of the main formula

The main body of the paper does not depend on this Appendix. Here we give another formulation of Theorem 2.1 in terms of shuffles of permutations for those who are interested in a more precise connection between the main formula and the shuffle product.

Let integers $k, \ell \geqslant 1$ be given. Let

$$\begin{aligned} S(k,\ell) :&= \{\sigma \in \Sigma_{k+\ell} \mid \sigma^{-1}(1) < \cdots < \sigma^{-1}(k), \sigma^{-1}(k+1) < \cdots < \sigma^{-1}(k+\ell)\} \\ &= \left\{ \sigma \in \Sigma_{k+\ell} \;\middle|\; \begin{array}{l} \text{if } 1 \leqslant \sigma(i) < \sigma(j) \leqslant k \\ \text{or } k+1 \leqslant \sigma(i) < \sigma(j) \leqslant k+\ell, \end{array} \ \text{then } i < j \right\}. \end{aligned} \tag{53}$$

be the set of (k, ℓ)-shuffles.

To state the shuffle form of our main formula we need the following notations. Define

$$\varepsilon_\sigma : [k+\ell] \to \{\pm 1\}, \quad \varepsilon_\sigma(i) = \begin{cases} 1, & 1 \leqslant \sigma(i) \leqslant k, \\ -1, & k+1 \leqslant \sigma(i) \leqslant k+\ell. \end{cases}$$

Let $\vec{r} = (r_1, \cdots, r_k) \in \mathbb{Z}^k_{\geqslant 1}$ and $\vec{s} = (s_1, \cdots, s_\ell) \in \mathbb{Z}^\ell_{\geqslant 1}$. Denote

$$\vec{\kappa} = (\kappa_1, \cdots, \kappa_{k+\ell}) := (r_1, \cdots, r_k, s_1, \cdots, s_\ell).$$

Let $\vec{a} \in G^k$ and $\vec{b} \in G^\ell$. Denote

$$\vec{\gamma} = (a_1, \cdots, a_k, b_1, \cdots, b_\ell).$$

For $\sigma \in S(k, \ell)$ we denote

$$\vec{a} ш_\sigma \vec{b} = (\gamma_{\sigma(1)}, \cdots \gamma_{\sigma(k+\ell)}).$$

We have the following equivalent form of Theorem 2.1.

Theorem 5.1. *Let G be a set and let $\mathcal{H}^{ш_\rho}(\widehat{G}) = (\mathcal{H}(\widehat{G}), ш_\rho)$ be as defined by Eq. (8). Then for $\left[{\vec{r} \atop \vec{a}} \right] \in \widehat{G}^k$ and $\left[{\vec{s} \atop \vec{b}} \right] \in \widehat{G}^\ell$ in $\mathcal{H}^{ш_\rho}(\widehat{G})$, we have*

$$\left[{\vec{r} \atop \vec{a}} \right] ш_\rho \left[{\vec{s} \atop \vec{b}} \right] = \sum_{\substack{\sigma \in S(k,\ell), \\ \vec{t} \in \mathbb{Z}^{k+\ell}_{\geqslant 1}, |\vec{t}| = |\vec{r}| + |\vec{s}|}} \left(\prod_{i=1}^{k+\ell} \binom{t_i - 1}{\kappa_{\sigma(i)} - 1 - \frac{1}{2}(1 - \varepsilon_\sigma(i)\varepsilon_\sigma(i-1)) \sum_{j=1}^{i-1} (t_j - \kappa_{\sigma(j)})} \right) \left[{\vec{t} \atop \vec{a} ш_\sigma \vec{b}} \right]$$

with the convention that $\varepsilon_\sigma(0) = \varepsilon_\sigma(1)$.

Proof. Let $\mathcal{I}_{k,\ell}$ be as defined in Eq. (16). We have the bijection between $S(k, \ell)$ and $\mathcal{I}_{k,\ell}$ given by

$$\sigma^{-1}(j) := \sigma^{-1}_{\varphi,\psi}(j) = \begin{cases} \varphi(j) & \text{if } 1 \leqslant j \leqslant k, \\ \psi(j-k) & \text{if } k+1 \leqslant j \leqslant k+\ell. \end{cases} \tag{54}$$

That is,

$$\sigma(i) := \sigma_{\varphi,\psi}(i) = \begin{cases} \varphi^{-1}(i) & \text{if } i \in \mathrm{im}(\varphi), \\ k + \psi^{-1}(i) & \text{if } i \in \mathrm{im}(\psi). \end{cases}$$

Thus we have

$$\kappa_{\sigma(i)} = \begin{cases} \kappa_{\varphi^{-1}(i)}, & i \in \mathrm{im}(\varphi) \\ \kappa_{k+\psi^{-1}(i)}, & i \in \mathrm{im}(\psi) \end{cases} = \begin{cases} r_{\varphi^{-1}(i)}, & i \in \mathrm{im}(\varphi) \\ s_{\psi^{-1}(i)}, & i \in \mathrm{im}(\psi) \end{cases} = h_{(\varphi,\psi),i} \tag{55}$$

and

$$(\vec{a} ш_\sigma \vec{b})_i = \gamma_{\sigma(i)} = \begin{cases} \gamma_{\varphi^{-1}(i)}, & i \in \mathrm{im}(\varphi) \\ \gamma_{k+\psi^{-1}(i)}, & i \in \mathrm{im}(\psi) \end{cases} = \begin{cases} a_{\varphi^{-1}(i)}, & i \in \mathrm{im}(\varphi) \\ b_{\psi^{-1}(i)}, & i \in \mathrm{im}(\psi) \end{cases} = (\vec{a} ш_{(\varphi,\psi)} \vec{b})_i. \tag{56}$$

By Eq. (56) we have

$$\vec{a} ш_\sigma \vec{b} = \vec{a} ш_{(\varphi,\psi)} \vec{b}. \tag{57}$$

Let $\varepsilon_{\varphi,\psi}$ be the function $[k+\ell] \to \{1,-1\}$ defined in Eq. (32). Then for $\sigma = \sigma_{\varphi,\psi}$,

$$\varepsilon_\sigma(i) = 1 \Leftrightarrow \sigma(i) \in [k] \Leftrightarrow i = \sigma^{-1}(j), j \in [k] \Leftrightarrow i = \varphi(j), j \in [k] \Leftrightarrow i \in \mathrm{im}(\varphi) \Leftrightarrow \varepsilon_{\varphi,\psi}(i) = 1.$$

So we have

$$\varepsilon_\sigma(i) = \varepsilon_{\varphi,\psi}(i), \qquad 1 \leqslant i \leqslant k+\ell. \tag{58}$$

Now our theorem follows from Eq. (33), (55), (57), (58) and Theorem 2.1. □

References

[1] D. Borwein, J. M. Borwein, and R. Girgensohn, Explicit evaluation of Euler sums, *Proc. Edinburgh Math. Soc. (2)* **38** (1995), 277-294.

[2] J. M. Borwein, D. M. Bradley and D. J. Broadhurst, Evaluations of k-fold Euler/Zagier Sums: A Compendium of Results for Arbitrary k, *Elec. J. Combin.*, **4** (1997), no. 2, #R5.

[3] J. M. Borwein, D. J. Broadhurst, D. M. Bradley, and P. Lisoněk, Special values of multiple polylogarithms, *Trans. Amer. Math. Soc.*, **353**, (2001), no. 3, 907–941.

[4] J. M. Borwein, D. J. Broadhurst, D. M. Bradley, and P. Lisoněk, Combinatorial aspects of multiple zeta values, Electron. J. Combin. 5 (1998), no. 1, Research Paper 38, 12.

[5] L. Boutet de Monvel, Remargues sur les Séries logarithmiques divergentes, Exposé au colloque “Polylogarithmes et conjecture de Deligne-Ihara” au C.I.R.M.(Luminy), April 2000.

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

[7] D. M. Bradley, Multiple q-zeta values, *J. Algebra*, **283**, (2005), no. 2, 752–798 `math.QA/0402093`

[8] D. M. Bradley, A q-analog of Euler’s decomposition formula for the double zeta function. *Int. J. Math. Math. Sci.* **21** (2005), 3453–3458.

[9] D. J. Broadhurst and D. Kreimer, Association of multiple zeta values with positive knots via Feynman diagrams up to 9 loops, *Phys. Lett. B*, **393**, (1997), no. 3-4, 403–412.

[10] D. J. Broadhurst, Massive 3-loop Feynman diagrams reducible to SC* primitives of algebras of the sixth root of unity, *European Phys. J. C (Fields)* **8** (1999), 311-333.

[11] P. Deligne and A. B. Goncharov, Groupes fondamentaux motiviques de Tate mixte, *Ann. Sci. École Norm. Sup.* **38** (2005), 1-56.

[12] M. Eie, W.-C. Liaw and Y. L. Ong, A restricted sum formula among multiple zeta values, *J. Number Theory*, to appear.

[13] H. Gangl, M. Kaneko, and D. Zagier, Double zeta values and modular forms, Automorphic forms and zeta functions, Proceedings of the conference in memory of Tsuneo Arakawa,World Sci. Publ., Hackensack, NJ (2006), 71-106.

[14] A.B. G. Goncharov, Multiple polylogarithms, cyclotomy and modular complexes, *Math. Res. Lett.* **5** (1998), 497-516.

[15] A. B. Goncharov, The Dihedral Lie Algebras and Galois Symmetries of $\pi_1^{(l)}(\mathbf{P} - (\{0,\infty\} \cup \mu_N))$, *Duke Math. J.* **110** (2001), 397-487.

[16] A. B. Goncharov and Y. Manin, Multiple ζ-motives and moduli spaces $\overline{\mathcal{M}}_{0,n}$, *Compos. Math.* **140** (2004), 1-14.

[17] A. Granville, A decomposition of Riemanns zeta-function, in: Analytic Number Theory, London Math. Soc. Lecture Note Ser., Vol. 247, Cambridge University Press, Cambridge, 1997, pp. 95-101.

[18] L. Guo, W. Keigher, Baxter algebras and shuffle products, *Adv. Math.*, **150**, (2000), 117-149.

[19] L. Guo and B. Xie, Structure theorems of mixable shuffle algebras and free commutative Rota-Baxter algebras, arXiv:0807:2267[math.RA].
[20] L. Guo and B. Xie, Weighted sum formula for multiple zeta values, axXiv:0809.5110[math.NT].
[21] L. Guo and B. Zhang, Renormalization of multiple zeta values, *J. Algebra*, **319** (2008), 3770-3809, arXiv:math.NT/0606076.
[22] L. Guo and B. Zhang, Differential Algebraic Birkhoff Decomposition and renormalization of multiple zeta values, *J. Number Theory*, **128** (2008), 2318-2339, arXiv:0710.0432(math.NT).
[23] M. E. Hoffman, Multiple harmonic series, *Pacific J. Math.*, **152** (1992), no. 2, 275–290.
[24] M. E. Hoffman, The algebra of multiple harmonic series, *J. Algebra*, **194**, no. 2, (1997), 477–495.
[25] M. E. Hoffman, Quasi-shuffle products, *J. Algebraic Combin.*, **11**, no. 1, (2000), 49–68.
[26] M. E. Hoffman and Y. Ohno, Relations of multiple zeta values and their algebraic expression. *J. Algebra* **262** (2003), 332–347.
[27] K. Ihara, M. Kaneko and D. Zagier, Derivation and double shuffle relations for multiple zeta values, *Compos. Math.* **142** (2006), 307–338.
[28] S. Kanemitsu, Y. Tanigawa, M. Yoshimoto, Convolution of Riemann zeta-values, *J. Math. Soc. Japan* **57** (2005), 1167–1177.
[29] C. Kassel, Quantum Groups, Springer, 1994.
[30] D. Manchon and S. Paycha, Renormalized Chen integrals for symbols on $\mathbb{R}^n$ and renormlized polyzeta functions, arXiv:math.NT/0604562.
[31] Y. Ohno, A generalization of the duality and sum formulas on the multiple zeta values, *J. Number Theory* **74** (1999), 39–43.
[32] Y. Ohno and J.-I. Okuda, On the sum formula for the q-analogue of non-strict multiple zeta values, *Proc. Amer. Math. Soc.* **135** (2007), 3029–3037.
[33] Y. Ohno and D. Zagier, Multiple zeta values of fixed weight, depth, and height, *Indag. Math. (N.S.)* **12** (2001), 483–487.
[34] Y. Ohno and W. Zudilin, Zeta stars, *Comm. Number Theory and Phys.* **2** (2008) 327-349.
[35] G. Racinet, Doubles mélanges des polylogarithmes multiples aux racines de l'unité, *Pub. Math. IHES*, **95** (2002), 185-231.
[36] C. Reutenauer, Free Lie Algebras, Oxford University Press, Oxford, UK, 1993.
[37] T. Terasoma, Mixed Tate motives and multiple zeta values, *Invent. Math.*, **149**, (2002), no. 2, 339–369. math.AG/0104231
[38] D. Zagier, Values of zeta functions and their applications, First European Congress of Mathematics, Vol. II (Paris, 1992), 497–512, *Progr. Math.*, **120**, Birkhuser, Basel, 1994
[39] D. Zagier, Multiple zeta values, preprint.
[40] J. Zhao, Multiple q-zeta functions and multiple q-polylogarithms. *Ramanujan J.* **14** (2007), 189–221
[41] J. Zhao, Double shuffle relations of Euler sum, arXiv:0705.2267[math.NT].

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