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# AN INTRODUCTION TO CLASSICAL AND FINITE MULTIPLE ZETA VALUES

*by*

Masanobu Kaneko

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**Abstract.** — We review some basic properties of multiple zeta values, in particular the theory of regularization and its connection to an identity between certain integral and series discovered in collaboration with S. Yamamoto. We also introduce the two “finite” versions of multiple zeta values, and a conjectural connection between them, which were discovered jointly with D. Zagier.

**Résumé.** — (*Une introduction aux valeurs des fonctions zétas multiples*) Nous décrivons certaines propriétés basiques des valeurs de fonctions zétas multiples. Nous explicitons en particulier la théorie des régularisations et son lien avec une identité, obtenue en collaboration avec S. Yamamoto, entre certaines intégrales et séries. Nous présentons également les deux versions « finies » des valeurs zétas multiples et un lien conjectural entre elles découvert conjointement avec D. Zagier.

## 1. Introduction

The multiple zeta value (MZV) is defined by the nested series

$$(1.1) \quad \zeta(k_1, \dots, k_r) = \sum_{0 < m_1 < \dots < m_r} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}},$$

where  $k_i$  ( $1 \leq i \leq r$ ) are arbitrary positive integers with  $k_r \geq 2$  (for convergence), and the sum is over  $r$  ordered positive integers.

The study of MZVs goes back to C. Goldbach and L. Euler, who investigated the case when  $r = 2$ . Since 1990’s, these numbers have appeared in a variety of branches of mathematics and mathematical physics as well, and a vast amount of work has been and still being done from various viewpoints and interests. In particular, it has turned out that *relations* among MZVs often reflected the structures of mathematical objects in various areas, and a great number of interesting relations have been found. However, we cannot yet say such and such relations describe *all* relations among MZVs, although several conjectural candidate sets of relations are known.

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The first part (from Section 2 to Section 6) of this expository article is devoted to review some basic properties of MZVs, and then explain the relation called the “extended double shuffle relations” and their connection to simpler, but equivalent “integral = series” type relations of S. Yamamoto and the author. In the second part (from Section 7 to Section 9), we explain about our joint work with D. Zagier on two types of “finite” analogues of classical multiple zeta values and their conjectural interrelation.

### 2. Definitions and the algebra of MZVs

Before discussing the multiple zeta *value*, we briefly mention the multiple zeta *function*

$$(2.1) \quad \zeta(s_1, \dots, s_r) = \sum_{0 < m_1 < \dots < m_r} \frac{1}{m_1^{s_1} \dots m_r^{s_r}}$$

of  $r$  complex variables  $s_i$ . About the region of convergence, the following was first stated and proved in [19].

**Proposition 2.1.** — *The series (2.1) is absolutely convergent in the region  $\Re(s_j + \dots + s_r) > r - j + 1$  ( $j = 1, 2, \dots, r$ ).*

*Proof.* — Set  $m_i := n_1 + \dots + n_i$  and  $\sigma_i := \Re(s_i)$ , and look at the series

$$\sum_{0 < m_1 < \dots < m_r} \left| \frac{1}{m_1^{s_1} \dots m_r^{s_r}} \right| = \sum_{n_1=1}^{\infty} \dots \sum_{n_r=1}^{\infty} \frac{1}{n_1^{\sigma_1} (n_1 + n_2)^{\sigma_2} \dots (n_1 + \dots + n_r)^{\sigma_r}}.$$

Using the simple estimate

$$\sum_{n=1}^{\infty} \frac{1}{(a+n)^\sigma} \leq \int_0^\infty \frac{1}{(a+x)^\sigma} dx = \frac{1}{\sigma-1} \frac{1}{a^{\sigma-1}}$$

for  $a > 0, \sigma > 1$ , we have, by the assumption  $\sigma_r > 1$ ,

$$\sum_{n_r=1}^{\infty} \frac{1}{(n_1 + \dots + n_r)^{\sigma_r}} \leq \frac{C}{(n_1 + \dots + n_{r-1})^{\sigma_r-1}}$$

with some positive constant  $C$ . Then, by  $\sigma_r + \sigma_{r-1} > 2$ , there exists a constant  $C' > 0$  such that

$$\begin{aligned} & \sum_{n_{r-1}=1}^{\infty} \sum_{n_r=1}^{\infty} \frac{1}{(n_1 + \dots + n_{r-1})^{\sigma_{r-1}}} \frac{1}{(n_1 + \dots + n_{r-1} + n_r)^{\sigma_r}} \\ & \leq \sum_{n_{r-1}=1}^{\infty} \frac{C}{(n_1 + \dots + n_{r-1})^{\sigma_{r-1} + \sigma_r - 1}} \leq \frac{C'}{(n_1 + \dots + n_{r-2})^{\sigma_{r-1} + \sigma_r - 2}} \end{aligned}$$

holds. We may proceed similarly and finally end up with the estimate

$$\sum_{0 < m_1 < \dots < m_r} \left| \frac{1}{m_1^{s_1} \dots m_r^{s_r}} \right| \leq \sum_{n_1=1}^{\infty} \frac{C''}{n_1^{\sigma_1 + \dots + \sigma_r - (r-1)}}$$

for some  $C'' > 0$ , and we are done because  $\sigma_1 + \dots + \sigma_r - (r - 1) > 1$ . □

**Theorem 2.2.** — The function  $\zeta(s_1, \dots, s_r)$  is meromorphically continued to the whole  $\mathbb{C}^r$ , with poles at

$$\begin{aligned} s_r &= 1, \\ s_r + s_{r-1} &= 2, 1, 0, -2, -4, -6, \dots \\ s_r + s_{r-1} + s_{r-2} &= 3, 2, 1, 0, -1, -2, -3, \dots (\in \mathbb{Z}_{\leq 3}) \\ &\vdots \\ s_r + \dots + s_1 &= r, r-1, \dots (\in \mathbb{Z}_{\leq r}). \end{aligned}$$

*Proof.* — We refer the reader e.g. [1] for a proof. □

Let us come back to the MZV, and we hereafter consider only positive integers as arguments in (1.1).

**Definition 2.3.** — For an index set  $\mathbf{k} = (k_1, \dots, k_r) \in \mathbb{N}^r$ , the quantities  $|\mathbf{k}| := k_1 + \dots + k_r$  and  $\text{dep}(\mathbf{k}) := r$  are respectively called *weight* and *depth*. When  $k_r > 1$ , the index  $\mathbf{k}$  is said to be *admissible*. By Proposition 2.1, the defining series (1.1) of the MZV converges if and only if  $\mathbf{k} = (k_1, \dots, k_r)$  is admissible. We often say the value  $\zeta(k_1, \dots, k_r)$  also has weight  $k = k_1 + \dots + k_r$  and depth  $r$ .

It is an easy exercise to see that the number of admissible indices of weight  $k$  and depth  $r$  is equal to  $\binom{k-2}{r-1}$ , and the total number of admissible indices of weight  $k$  is  $2^{k-2}$ .

	wt=2	wt=3	wt=4	wt=5
dep=1	$\zeta(2)$	$\zeta(3)$	$\zeta(4)$	$\zeta(5)$
dep=2		$\zeta(1, 2)$	$\zeta(1, 3), \zeta(2, 2)$	$\zeta(1, 4), \zeta(2, 3), \zeta(3, 2)$
dep=3			$\zeta(1, 1, 2)$	$\zeta(1, 1, 3), \zeta(1, 2, 2), \zeta(2, 1, 2)$
dep=4				$\zeta(1, 1, 1, 2)$

We introduce the  $\mathbb{Q}$ -vector space spanned by MZVs.

**Definition 2.4.** — We define the  $\mathbb{Q}$ -vector space  $\mathcal{Z}_k$  ( $k = 0, 1, 2, \dots$ ) as the subspace of  $\mathbb{R}$  spanned by MZVs of weight  $k$ :

$$\begin{aligned} \mathcal{Z}_0 &= \mathbb{Q}, \quad \mathcal{Z}_1 = \{0\}, \\ \mathcal{Z}_k &= \sum_{\substack{1 \leq r \leq k-1 \\ k_1, \dots, k_{r-1} \geq 1, k_r \geq 2 \\ k_1 + \dots + k_r = k}} \mathbb{Q} \cdot \zeta(k_1, \dots, k_r) \quad (k \geq 2). \end{aligned}$$

And further, put

$$\mathcal{Z} = \sum_{k=0}^{\infty} \mathcal{Z}_k.$$

Let us look at examples in small weights. There is only one element  $\zeta(2)$  of weight 2 and thus  $\mathcal{Z}_2 = \mathbb{Q} \cdot \zeta(2)$  (one dimensional). For weight 3, Euler’s famous identity  $\zeta(1, 2) = \zeta(3)$  shows that  $\mathcal{Z}_3 = \mathbb{Q} \cdot \zeta(1, 2) + \mathbb{Q} \cdot \zeta(3) = \mathbb{Q} \cdot \zeta(3)$  (one dimensional). We will see later that  $\mathcal{Z}_4$  is also one dimensional spanned by  $\zeta(4)$ . No value of  $k$  is known for which the dimension of  $\mathcal{Z}_k$  is strictly bigger than one, because of the difficulty to show the independence, for example of  $\zeta(5)$  and  $\zeta(2, 3)$  over  $\mathbb{Q}$ .

As for the dimension of  $\mathcal{Z}_k$ , the following remarkable conjecture of Zagier is widely known. Let the sequence  $d_k$  ( $k = 0, 1, 2, \dots$ ) be defined by the recursion

$$(2.2) \quad d_0 = 1, \quad d_1 = 0, \quad d_2 = 1, \quad d_k = d_{k-2} + d_{k-3} \quad (k \geq 3).$$

**Conjecture 2.5 (Zagier [38]).** — *We have  $\dim_{\mathbb{Q}} \mathcal{Z}_k = d_k$ .*

The ultimate upper bound result is established by A. Goncharov and T. Terasoma. As said above, no non-trivial lower bound is known so far.

**Theorem 2.6 (Goncharov [5], Terasoma [33], Deligne–Goncharov [4]).** — *We have  $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k$ .*

Below is the table of  $d_k$  and the total number ( $= 2^{k-2}$ ) of indices of weight  $k$ .

$k$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$d_k$	1	0	1	1	1	2	2	3	4	5	7	9	12	16	21	28
$2^{k-2}$	—	—	1	2	4	8	16	32	64	128	256	512	1024	2048	4096	8192

Note that the magnitude of  $d_k$  is far smaller than  $2^{k-2}$ , and hence we expect many relations among MZVs. What is the fundamental set of relations which is enough to deduce *all* relations? This is the basic question in the theory. There are several candidates of such a set: associator relations, extended (or regularized) double shuffle relations, Kawashima’s relations, etc.

The goal of the first part of this survey article is to introduce an elementary “integral-series relations” of Yamamoto and the author, and to explain its relation to the extended double shuffle relations.

We first show that the space  $\mathcal{Z}$  has a structure of a  $\mathbb{Q}$ -algebra.

**Proposition 2.7.** — *The space  $\mathcal{Z}$  is a  $\mathbb{Q}$ -algebra, and the multiplication respects weights, i.e.,  $\mathcal{Z}_k \cdot \mathcal{Z}_l \subset \mathcal{Z}_{k+l}$ .*

*Proof.* — There are at least two ways to prove this, one by using defining series (1.1) of MZVs, and the other using integral expressions. We introduce the integral expression in the next section, and here we give a proof using series.

For an integer  $N$ , let  $\zeta_N(k_1, \dots, k_r)$  be the truncated finite sum

$$(2.3) \quad \zeta_N(k_1, \dots, k_r) = \sum_{0 < m_1 < \dots < m_r < N} \frac{1}{m_1^{k_1} \dots m_r^{k_r}}.$$

When  $k_r > 1$ , this converges to  $\zeta(k_1, \dots, k_r)$  as  $N \rightarrow \infty$ .

For two indices  $\mathbf{k} = (k_1, \dots, k_r)$  and  $\mathbf{l} = (l_1, \dots, l_s)$ , we prove by induction on the sum  $r + s$  of depths that

$$\zeta_N(\mathbf{k})\zeta_N(\mathbf{l}) \text{ is a sum of } \zeta_N(\mathbf{m})\text{'s with some indices } \mathbf{m}\text{'s.}$$

When  $r + s = 2$ , i.e.,  $r = s = 1$ , this is true because

$$\begin{aligned}\zeta_N(k)\zeta_N(l) &= \sum_{0 < m < N} \frac{1}{m^k} \sum_{0 < n < N} \frac{1}{n^l} = \sum_{0 < m, n < N} \frac{1}{m^k n^l} \\ &= \left( \sum_{0 < m < n < N} + \sum_{0 < n < m < N} + \sum_{0 < m = n < N} \right) \frac{1}{m^k n^l} \\ &= \zeta_N(k, l) + \zeta_N(l, k) + \zeta_N(k + l).\end{aligned}$$

Let  $r + s > 2$  and suppose the assertion is true for the product of lesser sum of depths. We compute the product in a similar manner as

$$\begin{aligned}\zeta_N(\mathbf{k})\zeta_N(\mathbf{l}) &= \sum_{\substack{0 < m_1 < \dots < m_r < N \\ 0 < n_1 < \dots < n_s < N}} \frac{1}{m_1^{k_1} \dots m_r^{k_r} n_1^{l_1} \dots n_s^{l_s}} \\ &= \left( \sum_{\substack{0 < n_s < m_r < N \\ 0 < m_1 < \dots < m_r \\ 0 < n_1 < \dots < n_s}} + \sum_{\substack{0 < m_r < n_s < N \\ 0 < m_1 < \dots < m_r \\ 0 < n_1 < \dots < n_s}} + \sum_{\substack{0 < m_r = n_s < N \\ 0 < m_1 < \dots < m_r \\ 0 < n_1 < \dots < n_s}} \right) \frac{1}{m_1^{k_1} \dots m_r^{k_r} n_1^{l_1} \dots n_s^{l_s}} \\ &= \sum_{0 < m_r < N} \zeta_{m_r}(\mathbf{k}_-) \zeta_{m_r}(\mathbf{l}) \frac{1}{m_r^{k_r}} + \sum_{0 < n_s < N} \zeta_{n_s}(\mathbf{k}) \zeta_{n_s}(\mathbf{l}_-) \frac{1}{n_s^{l_s}} + \sum_{0 < m_r < N} \zeta_{m_r}(\mathbf{k}_-) \zeta_{m_r}(\mathbf{l}_-) \frac{1}{m_r^{k_r + l_s}},\end{aligned}$$

where  $\mathbf{k}_- = (k_1, \dots, k_{r-1})$ ,  $\mathbf{l}_- = (l_1, \dots, l_{s-1})$ , and  $\zeta_{\bullet}(\emptyset) = 1$ . By the induction hypothesis, the product  $\zeta_{m_r}(\mathbf{k}_-) \zeta_{m_r}(\mathbf{l})$  is a sum of  $\zeta_{m_r}(\mathbf{m})$ 's, and  $\sum_{0 < m_r < N} \zeta_{m_r}(\mathbf{m}) \frac{1}{m_r^{k_r}} = \zeta_N(\mathbf{m}, k_r)$ , and similarly for other two terms. This proves the assertion by induction. If both  $\mathbf{k}$  and  $\mathbf{l}$  are admissible, all  $\mathbf{m}$ 's that appear are clearly admissible. Hence by taking the limit  $N \rightarrow \infty$ , we obtain the first claim of the proposition. The second on weight is also clear from this computation.  $\square$

For later use, we introduce a formal space  $\mathcal{R}$  of indices, and equip  $\mathcal{R}$  with a product  $*$  coming from the above multiplication rule of MZVs in series form.

Let  $\mathcal{R} := \bigoplus_{r \geq 0} \mathbb{Q}[\mathbb{N}^r]$  be the space of finite  $\mathbb{Q}$ -linear combination of symbols  $[\mathbf{k}] = [k_1, \dots, k_r]$  with  $\mathbf{k} = (k_1, \dots, k_r) \in \mathbb{N}^r$ . We set  $\mathbb{Q}[\mathbb{N}^0] = \mathbb{Q}[\emptyset]$  and let  $\mathcal{R}^0$  be the subspace spanned by admissible (i.e.  $k_r \geq 2$ )  $[\mathbf{k}]$ 's. On  $\mathcal{R}$ , we define the “stuffle” (or harmonic, or quasi-shuffle) product  $*$  inductively by the following.

- It is  $\mathbb{Q}$ -bilinear,
- $[\emptyset] * [\mathbf{k}] = [\mathbf{k}] * [\emptyset] = [\mathbf{k}]$  for any  $\mathbf{k}$ ,
- $[\mathbf{k}] * [\mathbf{l}] = [[\mathbf{k}_-] * [\mathbf{l}], k_r] + [[\mathbf{k}] * [\mathbf{l}_-], l_s] + [[\mathbf{k}_-] * [\mathbf{l}_-], k_r + l_s]$ , where  $\mathbf{k} = (k_1, \dots, k_r)$ ,  $\mathbf{l} = (l_1, \dots, l_s)$ , and we put  $\mathbf{k}_- = (k_1, \dots, k_{r-1})$  and  $\mathbf{l}_- = (l_1, \dots, l_{s-1})$ .

Hoffman [9] shows that this product is associative and commutative. We write  $\mathcal{R}_*$  if we think of  $\mathcal{R}$  as a  $\mathbb{Q}$ -algebra with the product  $*$ . As is easily seen, the subspace  $\mathcal{R}^0$  becomes a subalgebra of  $\mathcal{R}_*$  and this subalgebra is denoted by  $\mathcal{R}_*^0$ . In the next section, we introduce another product  $\mathfrak{m}$  on  $\mathcal{R}$  coming from the integral expression of the MZV.

If we extend the association  $[\mathbf{k}] \mapsto \zeta(\mathbf{k})$   $\mathbb{Q}$ -linearly to the map  $\zeta : \mathcal{R}^0 \rightarrow \mathbb{R}$  (using the same letter  $\zeta$ ), then what we showed in the proof of Proposition 2.7 can be written as

$$(2.4) \quad \zeta(\mathbf{k})\zeta(\mathbf{l}) = \zeta([\mathbf{k}] * [\mathbf{l}])$$

for all admissible  $\mathbf{k}$  and  $\mathbf{l}$ , i.e., the  $\mathbb{Q}$ -linear map  $\zeta$  is an algebra homomorphism from  $\mathcal{R}_*^0$  to  $\mathbb{R}$ . We often write  $\zeta([\mathbf{k}] * [\mathbf{l}])$  as  $\zeta(\mathbf{k} * \mathbf{l})$  for notational simplicity.

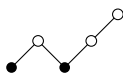
### 3. Integral expression

In this section, we review integral expressions of multiple zeta and multiple zeta-star values, by introducing a more general theory of Yamamoto on the integrals associated to 2-labeled posets [36].

**Definition 3.1.** — A 2-poset is a pair  $(X, \delta_X)$  of a finite partially ordered set (poset for short)  $X$  and a “label map”  $\delta_X$  from  $X$  to  $\{0, 1\}$ .

A 2-poset  $(X, \delta_X)$  is *admissible* if  $\delta_X(x) = 0$  for all maximal elements  $x \in X$  and  $\delta_X(x) = 1$  for all minimal elements  $x \in X$ .

It is convenient to use a Hasse diagram to describe a 2-poset, in which an element  $x$  with  $\delta_X(x) = 0$  (resp.  $\delta_X(x) = 1$ ) is represented by  $\circ$  (resp.  $\bullet$ ). For instance, the diagram



corresponds to the 2-poset  $X = \{x_1, x_2, x_3, x_4, x_5\}$  with the order  $x_1 < x_2 > x_3 < x_4 < x_5$  and label  $(\delta_X(x_1), \dots, \delta_X(x_5)) = (1, 0, 1, 0, 0)$ . This is an admissible 2-poset.

**Definition 3.2.** — For an admissible 2-poset  $X$ , we associate the integral

$$(3.1) \quad I(X) = \int_{\Delta_X} \prod_{x \in X} \omega_{\delta_X(x)}(t_x),$$

where

$$\Delta_X = \{(t_x)_x \in [0, 1]^X \mid t_x < t_y \text{ if } x < y\}$$

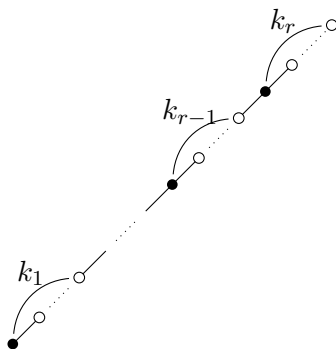
and

$$\omega_0(t) = \frac{dt}{t}, \quad \omega_1(t) = \frac{dt}{1-t}.$$

Note that the admissibility of a 2-poset ensures the convergence of the associated integral. When an admissible 2-poset is totally ordered, the corresponding integral is exactly the well-known iterated integral expression for a multiple zeta value. To be precise, for an index  $\mathbf{k} = (k_1, \dots, k_r)$ , we write



for the totally ordered diagram



If  $k_i = 1$ , we understand the notation



as a single  $\bullet$ , and if  $\mathbf{k} = \emptyset$ , we regard the diagram as the empty 2-poset.

**Theorem 3.3 (attributed to Kontsevich [38]).** — *If  $\mathbf{k}$  is an admissible index, we have*

$$(3.2) \quad \zeta(\mathbf{k}) = I \left( \textcircled{\bullet} \mathbf{k} \right) = \int_{0 < t_1 < \dots < t_{|\mathbf{k}|} < 1} \underbrace{\frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \dots \frac{dt_{k_1}}{t_{k_1}}}_{k_1} \dots \underbrace{\frac{dt_{|\mathbf{k}|-k_r+1}}{1-t_{|\mathbf{k}|-k_r+1}} \frac{dt_{|\mathbf{k}|-k_r+2}}{t_{|\mathbf{k}|-k_r+2}} \dots \frac{dt_{|\mathbf{k}|}}{t_{|\mathbf{k}|}}}_{k_r}.$$

An immediate corollary of this integral expression is an identity called “duality”. To describe this, first note that any admissible index can be written uniquely in the form

$$\mathbf{k} = (\underbrace{1, \dots, 1}_{a_1-1}, b_1 + 1, \dots, \underbrace{1, \dots, 1}_{a_h-1}, b_h + 1) \quad (a_i, b_i \geq 1).$$

The dual index  $\mathbf{k}^\dagger$  of  $\mathbf{k}$  is then given by

$$\mathbf{k}^\dagger = (\underbrace{1, \dots, 1}_{b_h-1}, a_h + 1, \dots, \underbrace{1, \dots, 1}_{b_1-1}, a_1 + 1),$$

and the duality of MZVs asserts that

$$\zeta(\mathbf{k}^\dagger) = \zeta(\mathbf{k}).$$

The proof is done by a simple change of variables  $t_i \rightarrow 1 - s_i$ .

Another corollary is a different product rule of MZVs. We only illustrate this by the simplest example  $\zeta(2)^2 = 2\zeta(2, 2) + 4\zeta(1, 3)$ . The integral expression of  $\zeta(2)$  is

$$\zeta(2) = \int_{0 < t_1 < t_2 < 1} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2}.$$



Multiplying and dividing the domain of integration, we obtain

$$\begin{aligned}
 \zeta(2)^2 &= \int_{0 < t_1 < t_2 < 1} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \int_{0 < s_1 < s_2 < 1} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} \\
 &= \int_{\substack{0 < t_1 < t_2 < 1 \\ 0 < s_1 < s_2 < 1}} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} \\
 &= \left( \int_{0 < t_1 < t_2 < s_1 < s_2 < 1} + \int_{0 < t_1 < s_1 < t_2 < s_2 < 1} + \int_{0 < s_1 < t_1 < t_2 < s_2 < 1} + \int_{0 < t_1 < s_1 < s_2 < t_2 < 1} \right. \\
 &\quad \left. + \int_{0 < s_1 < t_1 < s_2 < t_2 < 1} + \int_{0 < s_1 < s_2 < t_1 < t_2 < 1} \right) \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} \\
 &= \int_{0 < t_1 < t_2 < s_1 < s_2 < 1} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} + \int_{0 < t_1 < s_1 < t_2 < s_2 < 1} \frac{dt_1}{1-t_1} \frac{ds_1}{1-s_1} \frac{dt_2}{t_2} \frac{ds_2}{s_2} \\
 &\quad + \int_{0 < s_1 < t_1 < t_2 < s_2 < 1} \frac{ds_1}{1-s_1} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{ds_2}{s_2} + \int_{0 < t_1 < s_1 < s_2 < t_2 < 1} \frac{dt_1}{1-t_1} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} \frac{dt_2}{t_2} \\
 &\quad + \int_{0 < s_1 < t_1 < s_2 < t_2 < 1} \frac{ds_1}{1-s_1} \frac{dt_1}{1-t_1} \frac{ds_2}{s_2} \frac{dt_2}{t_2} + \int_{0 < s_1 < s_2 < t_1 < t_2 < 1} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \\
 &= \zeta(2, 2) + \zeta(1, 3) + \zeta(1, 3) + \zeta(1, 3) + \zeta(1, 3) + \zeta(2, 2) \\
 &= 2\zeta(2, 2) + 4\zeta(1, 3).
 \end{aligned}$$

The general case goes in exactly the same way, writing the Cartesian product of the simplices  $\{0 < t_1 < \dots < t_k < 1\} \times \{0 < s_1 < \dots < s_l < 1\}$  as a union of  $k + l$  dimensional simplices. We may formalize this product rule and define the shuffle product  $\mathfrak{m}$  on  $\mathcal{R}$ . For instance, the product  $[2]\mathfrak{m}[2] = 2[2, 2] + 4[1, 3]$  corresponds to the above example. The standard way to define  $\mathfrak{m}$  rigorously is to introduce the non-commutative algebra  $\mathbb{Q}\langle e_0, e_1 \rangle$  and transport the shuffle of words into a product of indices by assigning the word  $e_1 e_0^{k_1-1} \dots e_1 e_0^{k_r-1}$  to  $(k_1, \dots, k_r)$ . This association is the same as that of totally ordered poset, the correspondence being  $e_1 \leftrightarrow \bullet \leftrightarrow \frac{dt}{1-t}, e_0 \leftrightarrow \circ \leftrightarrow \frac{dt}{t}$ . See for example [35] for more detail.

We denote by  $\mathcal{R}_{\mathfrak{m}}$  and  $\mathcal{R}_{\mathfrak{m}}^0$  respectively the  $\mathbb{Q}$ -algebra  $(\mathcal{R}, \mathfrak{m})$  and its subalgebra  $(\mathcal{R}^0, \mathfrak{m})$ . The  $\mathbb{Q}$ -linear map  $\zeta : \mathcal{R}^0 \rightarrow \mathbb{R}$  is also an algebra homomorphism from  $\mathcal{R}_{\mathfrak{m}}^0$  to  $\mathbb{R}$ , i.e.,

$$(3.3) \quad \zeta(\mathbf{k})\zeta(\mathbf{l}) = \zeta([\mathbf{k}] \mathfrak{m} [\mathbf{l}])$$

(we often write the right-hand side as  $\zeta(\mathbf{k} \mathfrak{m} \mathbf{l})$ ) for any admissible indices  $\mathbf{k}$  and  $\mathbf{l}$ .

Combining the two products (2.4) and (3.3), we obtain the so-called (finite) double shuffle relations.

**Theorem 3.4 (finite double shuffle relation).** — *For any admissible indices  $\mathbf{k}$  and  $\mathbf{l}$ , we have*

$$\zeta(\mathbf{k} * \mathbf{l}) = \zeta(\mathbf{k} \mathfrak{m} \mathbf{l}).$$

We remark that the depth of any term in  $\mathbf{k} \mathfrak{m} \mathbf{l}$  is the sum of those of  $\mathbf{k}$  and  $\mathbf{l}$ , whereas  $\mathbf{k} * \mathbf{l}$  always contains the term with lesser depth. Therefore, the double shuffle relation always gives a non-trivial identity. For instance, if we take  $\mathbf{k} = \mathbf{l} = (2)$ , we have  $\zeta([2] * [2]) = 2\zeta(2, 2) + \zeta(4)$  and  $\zeta([2] \mathfrak{m} [2]) = 2\zeta(2, 2) + 4\zeta(1, 3)$ , and hence  $4\zeta(1, 3) = \zeta(4)$ .

Since the double shuffle relation comes from the product and the product respects the weight, the least weight of the relation obtained by the double shuffle relation is four. We cannot obtain Euler’s  $\zeta(1, 2) = \zeta(3)$  in this way. The theory of regularization remedies this deficiency.

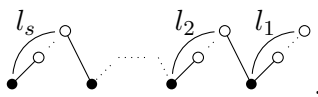
To have an idea, let us disregard the divergence for the moment and try to compute  $\zeta(1)\zeta(2)$  formally in two ways. By the  $*$ -product, we have  $\zeta(1)\zeta(2) = \zeta(1, 2) + \zeta(2, 1) + \zeta(3)$ , and by  $\mathfrak{m}$ , we have  $\zeta(1)\zeta(2) = 2\zeta(1, 2) + \zeta(2, 1)$  (compute  $\int_{0 < t < 1} \frac{dt}{1-t} \int_{0 < s_1 < s_2 < 1} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2}$  as above). Equating these, we see the divergent term  $\zeta(2, 1)$  cancels out and obtain  $\zeta(3) = \zeta(1, 2)$ . The theory of regularization explained in the next section makes this procedure rigorous. But before going into the next section, we give an integral expression of multiple zeta-star values. For an admissible index  $\mathbf{l} = (l_1, \dots, l_s)$ , the multiple zeta-star value (MZSV)  $\zeta^*(\mathbf{l})$  is defined by

$$\zeta^*(\mathbf{l}) = \sum_{0 < n_1 \leq \dots \leq n_s} \frac{1}{n_1^{l_1} \dots n_s^{l_s}}.$$

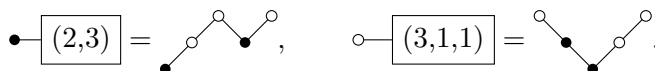
We set  $\zeta^*(\emptyset) = 1$ . For an index  $\mathbf{l} = (l_1, \dots, l_s)$ , we write



for the diagram



where the symbol  $\odot$  represents either  $\circ$  or  $\bullet$ . For example,



Note our convention in the case when some  $l_i$  is 1: the line from the  $\bullet$  corresponding to  $l_i = 1$  goes down (from left to right).

Then, if  $\mathbf{l}$  is an admissible index, we have

$$(3.4) \quad \zeta^*(\mathbf{l}) = I\left(\bullet \text{---} \boxed{\mathbf{l}}\right).$$

As an example, let us compute the simplest case  $\mathbf{l} = (1, 2)$ . The corresponding diagram is



$$\begin{aligned} I\left(\bullet \text{---} \circ\right) &= \int_{0 < t_1 < t_2 > t_3 > 0, t_2 < 1} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{dt_3}{1-t_3} = \int_{1 > t_2 > t_3 > 0} \sum_{n=1}^{\infty} \frac{t_2^n}{n} \frac{dt_2}{t_2} \frac{dt_3}{1-t_3} \\ &= \int_0^1 \sum_{n=1}^{\infty} \frac{1-t_3^n}{n^2} \frac{dt_3}{1-t_3} = \int_0^1 \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^n t_3^{m-1} dt_3 \\ &= \sum_{n > m \geq 1} \frac{1}{n^2 m} = \zeta^*(1, 2). \end{aligned}$$

Dividing the domain of integration according as  $t_1 < t_3$  and  $t_3 < t_1$ , we easily see that  $I\left(\bullet \text{---} \circ\right) = 2I\left(\bullet \text{---} \circ\right)$ , which implies  $\zeta^*(1, 2) = 2\zeta(1, 2)$ . On the other hand, we have  $\zeta^*(1, 2) = \zeta(1, 2) + \zeta(3)$  from the series expressions. Hence we deduce Euler's  $\zeta(1, 2) = \zeta(3)$ . This time we only used finite integral and the argument is completely rigorous.

We refer the reader to [36] for a proof of (3.4) in general, but it can be done similarly as above by repeated integrations from left to right.

### 4. Regularization and the extended double shuffle relation

In this section, we recall the theory of regularization of MZVs. The key fact is that both of the algebras  $\mathcal{R}_*$  and  $\mathcal{R}_{\text{III}}$  are freely generated by  $[1]$  over the subalgebras  $\mathcal{R}_*^0$  and  $\mathcal{R}_{\text{III}}^0$  respectively:

$$\mathcal{R}_* \simeq \mathcal{R}_*^0[[1]] \quad \text{and} \quad \mathcal{R}_{\text{III}} \simeq \mathcal{R}_{\text{III}}^0[[1]].$$

For proofs, see [9] and [24]. These isomorphisms assert that any element in  $\mathcal{R}$  can be written uniquely as a polynomial in the simplest divergent index  $[1]$  of weight 1 with admissible coefficients in  $\mathcal{R}_*$  and in  $\mathcal{R}_{\text{III}}$  respectively, examples being

$$\begin{aligned} [3, 1] &= [3] * [1] - [1, 3] - [4] \\ &= [3] \text{III} [1] - 2[1, 3] - [2, 2], \\ [2, 1, 1] &= \frac{1}{2}[2] * [1]^{*2} - ([1, 2] + [3]) * [1] + [1, 1, 2] + [1, 3] + \frac{1}{2}[4] \\ &= \frac{1}{2}[2] \text{III} [1]^{\text{III}2} - 2[1, 2] \text{III} [1] + 3[1, 1, 2]. \end{aligned}$$

Here,  $[1]^{*2} = [1] * [1]$ ,  $[1]^{\text{III}2} = [1] \text{III} [1]$ , and hereafter we use the notation  $[1]^{\bullet n}$  to denote  $\underbrace{[1] \bullet \cdots \bullet [1]}_{n \text{ times}}$  for  $\bullet = * \text{ or } \text{III}$ .

**Definition 4.1.** — For any index  $\mathbf{k}$ , write

$$[\mathbf{k}] = \sum_{i=0}^m a_i * [1]^{*i} \in \mathcal{R}_*^0[[1]] \quad (a_i \in \mathcal{R}^0)$$

and

$$[\mathbf{k}] = \sum_{j=0}^n b_j \text{III} [1]^{\text{III}j} \in \mathcal{R}_{\text{III}}^0[[1]] \quad (b_j \in \mathcal{R}^0).$$

Define  $*$ - and  $\text{III}$ -regularized polynomials  $\zeta_*(\mathbf{k}; T)$  and  $\zeta_{\text{III}}(\mathbf{k}; T)$  in  $\mathbb{R}[T]$  ( $T$ : indeterminate) respectively by

$$\zeta_*(\mathbf{k}; T) = \sum_{i=0}^m \zeta(a_i) T^i \quad \text{and} \quad \zeta_{\text{III}}(\mathbf{k}; T) = \sum_{j=0}^n \zeta(b_j) T^j.$$

When  $\mathbf{k}$  is admissible, we have  $\zeta_*(\mathbf{k}; T) = \zeta_{\text{III}}(\mathbf{k}; T) = \zeta(\mathbf{k})$ . The map  $\mathbf{k} \mapsto \zeta_*(\mathbf{k}; T)$  (resp.  $\mathbf{k} \mapsto \zeta_{\text{III}}(\mathbf{k}; T)$ ) is a unique homomorphism  $\mathcal{R}_* \rightarrow \mathbb{R}[T]$  (resp.  $\mathcal{R}_{\text{III}} \rightarrow \mathbb{R}[T]$ ) extending  $\zeta : \mathcal{R}_*^0 \rightarrow \mathbb{R}$  (resp.  $\zeta : \mathcal{R}_{\text{III}}^0 \rightarrow \mathbb{R}$ ) with  $\zeta_*([1]; T) = T$  (resp.  $\zeta_{\text{III}}([1]; T) = T$ ).

**Example 4.2.** — From the above, we have

$$\zeta_*(3, 1; T) = \zeta(3)T - \zeta(1, 3) - \zeta(4), \quad \zeta_{\text{III}}(3, 1; T) = \zeta(3)T - 2\zeta(1, 3) - \zeta(2, 2)$$

and

$$\begin{aligned} \zeta_*(2, 1, 1; T) &= \frac{1}{2}\zeta(2)T^2 - (\zeta(1, 2) + \zeta(3))T + \zeta(1, 1, 2) + \zeta(1, 3) + \frac{1}{2}\zeta(4), \\ \zeta_{\text{III}}(2, 1, 1; T) &= \frac{1}{2}\zeta(2)T^2 - \zeta(1, 2)T + 3\zeta(1, 1, 2). \end{aligned}$$

The fundamental theorem of regularizations of MZVs says that the two polynomials  $\zeta_{\mathfrak{m}}(\mathbf{k}; T)$  and  $\zeta_*(\mathbf{k}; T)$  are related with each other by a simple  $\mathbb{R}$ -linear map coming from the Taylor series of the gamma function  $\Gamma(z)$ . Define an  $\mathbb{R}$ -linear map  $\rho$  on  $\mathbb{R}[T]$  by the equality

$$(4.1) \quad \rho(e^{Tu}) = A(u)e^{Tu}$$

in the formal power series algebra  $\mathbb{R}[T][[u]]$  on which  $\rho$  acts coefficientwise, where

$$A(u) = \exp\left(\sum_{n=2}^{\infty} \frac{(-1)^n}{n} \zeta(n)u^n\right) \in \mathbb{R}[[u]].$$

Note that  $A(u) = e^{\gamma u} \Gamma(1 + u)$ , where  $\gamma$  is Euler's constant.

**Example 4.3.** — Since we have

$$A(u) = 1 + \zeta(2)\frac{u^2}{2} - 2\zeta(3)\frac{u^3}{3!} + (6\zeta(4) + 3\zeta(2)^2)\frac{u^4}{4!} + \dots,$$

multiplying

$$e^{Tu} = 1 + Tu + T^2\frac{u^2}{2!} + T^3\frac{u^3}{6} + T^4\frac{u^4}{24} + \dots$$

we find

$$\begin{aligned} \rho(1) &= 1, \\ \rho(T) &= T, \\ \rho(T^2) &= T^2 + \zeta(2), \\ \rho(T^3) &= T^3 + 3\zeta(2)T - 2\zeta(3), \\ \rho(T^4) &= T^4 + 6\zeta(2)T^2 - 8\zeta(3)T + 6\zeta(4) + 3\zeta(2)^2. \end{aligned}$$

**Theorem 4.4** ([11, Theorem 1]). — *For any index  $\mathbf{k}$ , we have*

$$(4.2) \quad \zeta_{\mathfrak{m}}(\mathbf{k}; T) = \rho(\zeta_*(\mathbf{k}; T)).$$

It is conjectured that this relation (or more precisely the relations obtained by comparing the coefficients), together with the double shuffle relations

$$(4.3) \quad \zeta(\mathbf{k})\zeta(\mathbf{l}) = \zeta(\mathbf{k} * \mathbf{l}) = \zeta(\mathbf{k} \mathfrak{m} \mathbf{l})$$

describes all (algebraic and linear) relations of MZVs over  $\mathbb{Q}$ . These relations as a whole are referred to as the extended (or regularized) double shuffle relations. For a complete set of *linear* relations, it is conjectured in [11] that either

$$\zeta_*(\mathbf{k} * \mathbf{l} - \mathbf{k} \mathfrak{m} \mathbf{l}; 0) = 0 \quad (\forall \mathbf{k} \in \mathcal{R}^0 \text{ and } \forall \mathbf{l} \in \mathcal{R})$$

or

$$\zeta_{\mathfrak{m}}(\mathbf{k} * \mathbf{l} - \mathbf{k} \mathfrak{m} \mathbf{l}; 0) = 0 \quad (\forall \mathbf{k} \in \mathcal{R}^0 \text{ and } \forall \mathbf{l} \in \mathcal{R})$$

gives such a set. These too are sometimes called the extended double shuffle relations. For instance, if we take  $\mathbf{k} = (2)$  and  $\mathbf{l} = (1)$ , we have

$$\mathbf{k} * \mathbf{l} - \mathbf{k} \mathfrak{m} \mathbf{l} = [3] - [1, 2]$$

and so

$$\zeta_*(\mathbf{k} * \mathbf{l} - \mathbf{k} \mathfrak{m} \mathbf{l}; T) = \zeta_{\mathfrak{m}}(\mathbf{k} * \mathbf{l} - \mathbf{k} \mathfrak{m} \mathbf{l}; T) = \zeta(3) - \zeta(1, 2).$$

This gives  $\zeta(3) = \zeta(1, 2)$ . Further, if we take  $\mathbf{k} = (2)$  and  $\mathbf{l} = (1, 1)$ , we have

$$\mathbf{k} * \mathbf{l} - \mathbf{k} \text{ m } \mathbf{l} = [1, 3] + [3, 1] - 2[1, 1, 2] - [1, 2, 1].$$

A little computation shows

$$\zeta_*(\mathbf{k} * \mathbf{l} - \mathbf{k} \text{ m } \mathbf{l}; T) = (\zeta(3) - \zeta(1, 2))T - \zeta(4) + \zeta(1, 3) + \zeta(2, 2)$$

and

$$\zeta_{\text{m}}(\mathbf{k} * \mathbf{l} - \mathbf{k} \text{ m } \mathbf{l}; T) = (\zeta(3) - \zeta(1, 2))T - \zeta(1, 3) - \zeta(2, 2) + \zeta(1, 1, 2).$$

Therefore, from  $\zeta_*(\mathbf{k} * \mathbf{l} - \mathbf{k} \text{ m } \mathbf{l}; 0) = 0$  we have  $\zeta(1, 3) + \zeta(2, 2) = \zeta(4)$  and from  $\zeta_{\text{m}}(\mathbf{k} * \mathbf{l} - \mathbf{k} \text{ m } \mathbf{l}; 0) = 0$  we have  $\zeta(1, 3) + \zeta(2, 2) = \zeta(1, 1, 2)$ . These relations together with  $4\zeta(1, 3) = \zeta(4)$  obtained after Theorem 3.4 (finite double shuffle relation) give  $\zeta(1, 3) = \frac{1}{4}\zeta(4)$ ,  $\zeta(2, 2) = \frac{3}{4}\zeta(4)$ ,  $\zeta(1, 1, 2) = \zeta(4)$ , and thus we conclude  $\mathcal{Z}_4 = \mathbb{Q} \cdot \zeta(4)$ .

### 5. Integral-series identity

For a non-empty index  $\mathbf{k} = (k_1, \dots, k_r)$ , we write  $\mathbf{k}^*$  for the formal sum of  $2^{r-1}$  indices of the form  $(k_1 \circ \dots \circ k_r)$ , where each  $\circ$  is replaced by “ $\cdot$ ”, “ $+$ ” or “ $+$ ”. We also put  $\emptyset^* = \emptyset$ . Then  $\mathbf{k}^*$  is identified with an element of  $\mathcal{R}$ , and we have  $\zeta^*(\mathbf{k}) = \zeta(\mathbf{k}^*)$  for admissible  $\mathbf{k}$ .

We introduce the  $\mathbb{Q}$ -bilinear “circled stuffle product”  $\otimes: (\mathcal{R} \setminus \mathbb{Q}[\emptyset]) \times (\mathcal{R} \setminus \mathbb{Q}[\emptyset]) \rightarrow \mathcal{R}^0$  defined by

$$[\mathbf{k}_-, k_r] \otimes [\mathbf{l}_-, l_s] = [\mathbf{k}_- * \mathbf{l}_-, k_r + l_s] \quad (\mathbf{k}_-, \mathbf{l}_- \in \mathcal{R}, k_r, l_s \geq 1).$$

We readily see from the definition that, for non-empty indices  $\mathbf{k} = (k_1, \dots, k_r)$  and  $\mathbf{l} = (l_1, \dots, l_s)$ , we have the series expression

$$(5.1) \quad \zeta(\mathbf{k} \otimes \mathbf{l}^*) = \sum_{0 < m_1 < \dots < m_r = n_s \geq \dots \geq n_1 > 0} \frac{1}{m_1^{k_1} \dots m_r^{k_r} n_1^{l_1} \dots n_s^{l_s}}.$$

To see this, we put  $n = m_r (= n_s)$  and write the right-hand side as

$$\sum_{n=1}^{\infty} \left( \sum_{0 < m_1 < \dots < m_{r-1} < n} \frac{1}{m_1^{k_1} \dots m_{r-1}^{k_{r-1}}} \right) \left( \sum_{0 < n_1 \leq \dots \leq n_{s-1} \leq n} \frac{1}{n_1^{l_1} \dots n_{s-1}^{l_{s-1}}} \right) \frac{1}{n^{k_r + l_s}},$$

and note that the product of truncated sums for a fixed  $n$  obey the stuffle product rule, as seen in the proof of Proposition 2.7.

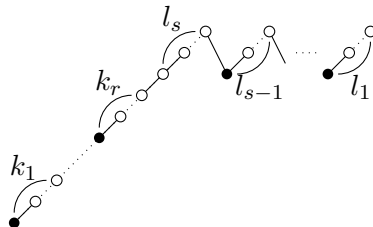
The formula (5.1) includes MZV and MZSV as special cases:

$$\zeta(\mathbf{k} \otimes (1)^*) = \zeta(k_1, \dots, k_{r-1}, k_r + 1)$$

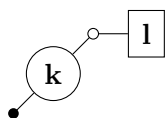
and

$$\zeta((1) \otimes \mathbf{l}^*) = \zeta^*(l_1, \dots, l_{s-1}, l_s + 1).$$

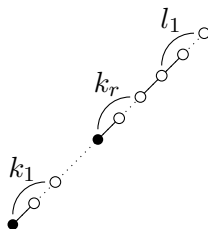
For non-empty indices  $\mathbf{k} = (k_1, \dots, k_r)$  and  $\mathbf{l} = (l_1, \dots, l_s)$ , the diagram



is denoted by



This is a combination of the symbols introduced in Section 3 for integral expressions of  $\zeta(\mathbf{k})$  and  $\zeta^*(\mathbf{l})$ . When  $s = 1$ , we understand this as



In [17], we proved the following identity which generalizes both (3.2) and (3.4).

**Theorem 5.1.** — For any non-empty indices  $\mathbf{k}$  and  $\mathbf{l}$ , we have

$$(5.2) \quad I \left( \begin{array}{c} \square \mathbf{l} \\ \circ \\ \text{---} \\ \circ \mathbf{k} \end{array} \right) = \zeta(\mathbf{k} \otimes \mathbf{l}^*).$$

The proof is done by a straightforward calculation of the multiple integral as a repeated integral from left to right. The following example is taken from [17].

**Example 5.2.** — Take  $\mathbf{k} = (1, 1)$  and  $\mathbf{l} = (2, 1)$ . Then, omitting the condition  $0 < t_i < 1$  from the notation, we have

$$\begin{aligned} I \left( \begin{array}{c} \circ \\ \text{---} \\ \circ \\ \text{---} \\ \circ \end{array} \right) &= \int_{t_1 < t_2 < t_3 > t_4 < t_5} \frac{dt_1}{1-t_1} \frac{dt_2}{1-t_2} \frac{dt_3}{t_3} \frac{dt_4}{1-t_4} \frac{dt_5}{t_5} \\ &= \int_{t_2 < t_3 > t_4 < t_5} \sum_{l=1}^{\infty} \frac{t_2^l}{l} \frac{dt_2}{1-t_2} \frac{dt_3}{t_3} \frac{dt_4}{1-t_4} \frac{dt_5}{t_5} \\ &= \int_{t_3 > t_4 < t_5} \sum_{l,m=1}^{\infty} \frac{t_3^{l+m}}{l(l+m)} \frac{dt_3}{t_3} \frac{dt_4}{1-t_4} \frac{dt_5}{t_5} \\ &= \int_{t_4 < t_5} \sum_{l,m=1}^{\infty} \frac{1-t_4^{l+m}}{l(l+m)^2} \frac{dt_4}{1-t_4} \frac{dt_5}{t_5} \\ &= \int_{t_4 < t_5} \sum_{0 < m_1 < m_2} \frac{1}{m_1 m_2^2} \sum_{n=1}^{m_2} t_4^{n-1} dt_4 \frac{dt_5}{t_5} \\ &= \int_0^1 \sum_{0 < m_1 < m_2} \frac{1}{m_1 m_2^2} \sum_{n=1}^{m_2} \frac{t_5^n}{n} \frac{dt_5}{t_5} \\ &= \sum_{0 < m_1 < m_2 \geq n > 0} \frac{1}{m_1 m_2^2 n^2} = \sum_{0 < m_1 < m_2 = n_2 \geq n_1 > 0} \frac{1}{m_1 m_2 n_1^2 n_2} \\ &= \zeta(\mathbf{k} \otimes \mathbf{l}^*). \end{aligned}$$



**Proposition 6.1.** — Let  $\tilde{I}_*$  and  $\tilde{J}_*$  be  $*$ -ideals of  $\mathcal{R}_*^0$  generated respectively by  $I_*$  and  $J$ . Similarly let  $\tilde{I}_{\text{III}}$  and  $\tilde{J}_{\text{III}}$  be  $\text{III}$ -ideals of  $\mathcal{R}_{\text{III}}^0$  generated by  $I_{\text{III}}$  and  $J$ . Then these four ideals are identical as sets:

$$\tilde{I}_* = \tilde{J}_* = \tilde{I}_{\text{III}} = \tilde{J}_{\text{III}}.$$

*Proof.* — We freely use identities proved in [17]. From equations  $(A_{\text{III}}), (A_*)$  in Lemma 5.2 of [17], we have

$$(6.1) \quad \sum_{i=0}^{s-1} (-1)^i \mu(\mathbf{k}, \mathbf{l}^i) \text{III } \overleftarrow{\mathbf{l}}_i = \sum_{i=0}^{s-1} (-1)^i (\mathbf{k} \otimes (\mathbf{l}^i)^*) * \overleftarrow{\mathbf{l}}_i.$$

Here,  $\mathbf{k}, \mathbf{l}$  are non-empty indices,  $\mathbf{l}^i$  and  $\overleftarrow{\mathbf{l}}_i$  are indices obtained by dropping and taking the first  $i$  components of  $\mathbf{l}$  respectively, and  $\overleftarrow{\mathbf{l}}_i$  is the reversal of the index  $\mathbf{l}_i$ . By separating the terms for  $i = 0$ , we obtain

$$(6.2) \quad \mu(\mathbf{k}, \mathbf{l}) - \mathbf{k} \otimes \mathbf{l}^* = \sum_{i=1}^{s-1} (-1)^i \left( (\mathbf{k} \otimes (\mathbf{l}^i)^*) * \overleftarrow{\mathbf{l}}_i - \mu(\mathbf{k}, \mathbf{l}^i) \text{III } \overleftarrow{\mathbf{l}}_i \right),$$

which can be written as

$$\mu(\mathbf{k}, \mathbf{l}) - \mathbf{k} \otimes \mathbf{l}^* = \sum_{i=1}^{s-1} (-1)^i \left( (\mathbf{k} \otimes (\mathbf{l}^i)^* - \mu(\mathbf{k}, \mathbf{l}^i)) * \overleftarrow{\mathbf{l}}_i + \mu(\mathbf{k}, \mathbf{l}^i) * \overleftarrow{\mathbf{l}}_i - \mu(\mathbf{k}, \mathbf{l}^i) \text{III } \overleftarrow{\mathbf{l}}_i \right).$$

Take  $\text{reg}_*$  of both sides. Setting  $j(\mathbf{k}, \mathbf{l}) := \mu(\mathbf{k}, \mathbf{l}) - \mathbf{k} \otimes \mathbf{l}^*$  and noticing this is an element in  $\mathcal{R}^0$  (and hence unchanged by taking  $\text{reg}_*$ ), we may conclude by induction on the length of  $\mathbf{l}$  that  $j(\mathbf{k}, \mathbf{l}) \in \tilde{I}_*$ . In fact, if the length of  $\mathbf{l}$  is 0, then  $j(\mathbf{k}, \mathbf{l}) = 0$  and the assertion is trivial. If the length of  $\mathbf{l}$  is  $s \geq 1$ , then the length of  $\mathbf{l}^i$  is  $s - i$  and the induction hypothesis gives

$$\text{reg}_*((\mathbf{k} \otimes (\mathbf{l}^i)^* - \mu(\mathbf{k}, \mathbf{l}^i)) * \overleftarrow{\mathbf{l}}_i) = (\mathbf{k} \otimes (\mathbf{l}^i)^* - \mu(\mathbf{k}, \mathbf{l}^i)) * \text{reg}_*(\overleftarrow{\mathbf{l}}_i) \in \tilde{I}_*$$

(this is because  $\text{reg}_*$  is a  $*$ -homomorphism,  $\mathbf{k} \otimes (\mathbf{l}^i)^* - \mu(\mathbf{k}, \mathbf{l}^i) \in \mathcal{R}^0$ , and  $\text{reg}_*(\mu(\mathbf{k}, \mathbf{l}^i) * \overleftarrow{\mathbf{l}}_i - \mu(\mathbf{k}, \mathbf{l}^i) \text{III } \overleftarrow{\mathbf{l}}_i) \in I_*$ ). Hence we have  $J \subseteq \tilde{I}_*$  and  $\tilde{J}_* \subseteq \tilde{I}_*$ . Likewise, writing (6.2) as

$$\mu(\mathbf{k}, \mathbf{l}) - \mathbf{k} \otimes \mathbf{l}^* = \sum_{i=1}^{s-1} (-1)^i \left( (\mathbf{k} \otimes (\mathbf{l}^i)^*) * \overleftarrow{\mathbf{l}}_i - (\mathbf{k} \otimes (\mathbf{l}^i)^*) \text{III } \overleftarrow{\mathbf{l}}_i + (\mathbf{k} \otimes (\mathbf{l}^i)^* - \mu(\mathbf{k}, \mathbf{l}^i)) \text{III } \overleftarrow{\mathbf{l}}_i \right)$$

and taking  $\text{reg}_{\text{III}}$  of both sides, we obtain  $\tilde{J}_{\text{III}} \subseteq \tilde{I}_{\text{III}}$ .

Next, let  $\mathbf{k} = (k_1, \dots, k_r)$  be an admissible index and  $\mathbf{l} = (l_1, \dots, l_s)$  be any index. Replace  $\mathbf{k}$  and  $\mathbf{l}$  in (6.1) by  $\tilde{\mathbf{k}} = (k_1, \dots, k_{r-1}, k_r - 1)$  and  $\hat{\mathbf{l}} = (l_s, \dots, l_1, 1)$  respectively. Then we have

$$\sum_{i=0}^s (-1)^i \mu(\tilde{\mathbf{k}}, \hat{\mathbf{l}}^i) \text{III } \mathbf{l}^{s-i} = \sum_{i=0}^s (-1)^i (\tilde{\mathbf{k}} \otimes (\hat{\mathbf{l}}^i)^*) * \mathbf{l}^{s-i},$$

and by separating the terms for  $i = s$  and multiplying  $(-1)^s$ , we have

$$(6.3) \quad \mathbf{k} * \mathbf{l} - \mathbf{k} \text{III } \mathbf{l} = \sum_{i=0}^{s-1} (-1)^{s-i} \left( \mu(\tilde{\mathbf{k}}, \hat{\mathbf{l}}^i) \text{III } \mathbf{l}^{s-i} - (\tilde{\mathbf{k}} \otimes (\hat{\mathbf{l}}^i)^*) * \mathbf{l}^{s-i} \right).$$

Write this as

$$\mathbf{k} * \mathbf{l} - \mathbf{k} \text{III } \mathbf{l} = \sum_{i=0}^{s-1} (-1)^{s-i} \left( \mu(\tilde{\mathbf{k}}, \hat{\mathbf{l}}^i) \text{III } \mathbf{l}^{s-i} - \mu(\tilde{\mathbf{k}}, \hat{\mathbf{l}}^i) * \mathbf{l}^{s-i} + (\mu(\tilde{\mathbf{k}}, \hat{\mathbf{l}}^i) - (\tilde{\mathbf{k}} \otimes (\hat{\mathbf{l}}^i)^*)) * \mathbf{l}^{s-i} \right),$$



and take  $\text{reg}_*$  of both sides to conclude  $\widetilde{I}_* \subseteq \widetilde{J}_*$  by induction on the length of  $\mathbf{l}$ . Similarly, write

$$\mathbf{k} * \mathbf{l} - \mathbf{k} \text{III} \mathbf{l} = \sum_{i=0}^{s-1} (-1)^{s-i} \left( (\mu(\widehat{\mathbf{k}}, \widehat{\mathbf{l}}^i) - \widehat{\mathbf{k}} \otimes (\widehat{\mathbf{l}}^i)^*) \text{III} \mathbf{l}^{s-i} + (\widehat{\mathbf{k}} \otimes (\widehat{\mathbf{l}}^i)^*) \text{III} \mathbf{l}^{s-i} - (\widehat{\mathbf{k}} \otimes (\widehat{\mathbf{l}}^i)^*) * \mathbf{l}^{s-i} \right)$$

and take  $\text{reg}_{\text{III}}$  to obtain  $\widetilde{I}_{\text{III}} \subseteq \widetilde{J}_{\text{III}}$ . Therefore, we have  $\widetilde{I}_* = \widetilde{J}_*$  and  $\widetilde{I}_{\text{III}} = \widetilde{J}_{\text{III}}$ .

Finally, for  $\mathbf{m} \in \mathcal{R}^0$  and  $j(\mathbf{k}, \mathbf{l}) \in J(\subseteq \mathcal{R}^0)$ , we have  $\mathbf{m} * j(\mathbf{k}, \mathbf{l}) - \mathbf{m} \text{III} j(\mathbf{k}, \mathbf{l}) \in \widetilde{J}_{\text{III}}$  by  $I_{\text{III}} \subseteq \widetilde{J}_{\text{III}}$  and hence  $\mathbf{m} * j(\mathbf{k}, \mathbf{l}) \in \widetilde{J}_{\text{III}}$ , i.e.,  $\widetilde{J}_* \subseteq \widetilde{J}_{\text{III}}$ . The same argument implies  $\widetilde{J}_{\text{III}} \subseteq \widetilde{J}_*$  and we conclude  $\widetilde{J}_* = \widetilde{J}_{\text{III}}$ . Thus we are done.  $\square$

### 7. $\mathcal{A}$ -finite multiple zeta values

Consider the ring  $\mathcal{A}$  defined by

$$\mathcal{A} := \frac{\prod_p \mathbb{Z}/p\mathbb{Z}}{\bigoplus_p \mathbb{Z}/p\mathbb{Z}} = \{(a_{(p)})_p \mid a_{(p)} \in \mathbb{Z}/p\mathbb{Z}\} / \sim.$$

Here,  $p$  runs over all prime numbers, and the relation  $(a_{(p)})_p \sim (b_{(p)})_p$  indicates that the equality  $a_{(p)} = b_{(p)}$  in  $\mathbb{Z}/p\mathbb{Z}$  holds for all large enough  $p$ . Component-wise addition and multiplication equip  $\mathcal{A}$  with the structure of a ring. Moreover, the well-defined injective map  $\mathbb{Q} \ni r \mapsto (r \bmod p)_p \in \mathcal{A}$  makes  $\mathcal{A}$  into a  $\mathbb{Q}$ -algebra. Alternatively,  $\mathcal{A}$  is isomorphic to  $(\prod_p \mathbb{Z}/p\mathbb{Z}) \otimes_{\mathbb{Z}} \mathbb{Q}$  or  $\prod_p \mathbb{Z}/p\mathbb{Z}$  modulo torsion. We often identify a representative  $a = (a_{(p)})_p$  with the element in  $\mathcal{A}$  that it defines, where  $a_{(p)}$  denotes the  $p$ -component of  $a$ .

**Definition 7.1.** — For an index  $\mathbf{k} = (k_1, \dots, k_r)$ , define the  $\mathcal{A}$ -finite multiple zeta value  $\zeta^{\mathcal{A}}(\mathbf{k}) = \zeta^{\mathcal{A}}(k_1, \dots, k_r) \in \mathcal{A}$  by

$$(7.1) \quad \zeta^{\mathcal{A}}(k_1, \dots, k_r)_{(p)} = \sum_{0 < m_1 < \dots < m_r < p} \frac{1}{m_1^{k_1} \dots m_r^{k_r}} \pmod{p}.$$

With the notation adopted in (2.3), the right-hand side is written as  $\zeta_p(\mathbf{k}) \pmod{p}$ .

Similarly as in the case of ordinary real MZVs, we are interested in the  $\mathbb{Q}$ -vector space in  $\mathcal{A}$  spanned by  $\zeta^{\mathcal{A}}(k_1, \dots, k_r)$ .

**Definition 7.2.** — For each integer  $k \geq 0$ , define the  $\mathbb{Q}$ -vector space  $\mathcal{Z}_{\mathcal{A},k} \subseteq \mathcal{A}$  by  $\mathcal{Z}_{\mathcal{A},0} = \mathbb{Q}$  and

$$\mathcal{Z}_{\mathcal{A},k} := \sum_{\substack{k_1 + \dots + k_r = k \\ r \geq 1, k_i \geq 1}} \mathbb{Q} \cdot \zeta^{\mathcal{A}}(k_1, \dots, k_r) \quad (k \geq 1).$$

Further, we set

$$\mathcal{Z}_{\mathcal{A}} := \sum_{k=0}^{\infty} \mathcal{Z}_{\mathcal{A},k}.$$

Although components  $k_i$  of an index may be 0 or negative because there is no convergence issue in this setting, we restrict ourselves to positive integer components. In fact, it can be easily seen that the space  $\mathcal{Z}_{\mathcal{A}}$  does not enlarge if we allow non-positive components. For instance, we see

$$\zeta^{\mathcal{A}}(-1, 3, 2) = \frac{1}{2} \zeta^{\mathcal{A}}(1, 2) - \frac{1}{2} \zeta^{\mathcal{A}}(2, 2)$$

by using the Seki–Bernoulli formula for sum of powers. However, the notion of weight does not behave well if there is a non-positive component, as the above example indicates. Since the stuffle relation like

$$\zeta^{\mathcal{A}}(k_1)\zeta^{\mathcal{A}}(k_2) = \zeta^{\mathcal{A}}(k_1, k_2) + \zeta^{\mathcal{A}}(k_2, k_1) + \zeta^{\mathcal{A}}(k_1 + k_2)$$

holds for  $\zeta^{\mathcal{A}}(\mathbf{k})$  (this is because the finite truncation  $\zeta_p(\mathbf{k})$  satisfies the stuffle product rule as shown in the proof of Proposition 2.7), the space  $\mathcal{Z}_{\mathcal{A}}$  is a  $\mathbb{Q}$ -algebra. As for the dimension of each  $\mathcal{Z}_{\mathcal{A},k}$ , again Zagier numerically observed

**Conjecture 7.3.** — *Let  $d_k$  be the sequence defined in (2.2). Then we would have*

$$\dim_{\mathbb{Q}} \mathcal{Z}_{\mathcal{A},k} = d_{k-3} \quad (= d_k - d_{k-2}) \quad (\forall k).$$

This is in accordance with our “main conjecture”

$$\mathcal{Z}_{\mathcal{A}} \simeq \mathcal{Z}/\zeta(2)\mathcal{Z},$$

where  $\mathcal{Z}$  is the  $\mathbb{Q}$ -algebra of classical MZVs. If Conjecture 2.5 is true and the weight gives a grading on  $\mathcal{Z}$ , then the weight  $k$  piece of  $\mathcal{Z}/\zeta(2)\mathcal{Z}$  should have dimension  $d_k - d_{k-2} = d_{k-3}$ . We shall state the main conjecture in a more precise form in Section 9. Let us look at some examples of  $\zeta_{\mathcal{A}}(\mathbf{k})$  in low depths.

**Example 7.4.** —

(1) Depth 1 case: If  $k \neq 0$ , then  $\zeta^{\mathcal{A}}(k) = 0$ . This is because we have

$$\sum_{0 < m < p} \frac{1}{m^k} \equiv 0 \pmod{p}$$

when  $p - 1 \nmid k$ , and for a fixed  $k$  this is satisfied by all  $p$  greater than  $k + 1$ . For  $k = 0$ , we obviously have  $\zeta^{\mathcal{A}}(0) = -1$ .

(2) Depth 2 case: We have

$$(7.2) \quad \zeta^{\mathcal{A}}(k_1, k_2) = (-1)^{k_2} \binom{k_1 + k_2}{k_1} Z(k_1 + k_2) \quad (\forall k_1, k_2 \geq 1).$$

Here, for  $k \geq 2$ , the element  $Z(k) \in \mathcal{A}$  is defined by setting its  $p$ -component as

$$Z(k)_{(p)} = \frac{B_{p-k}}{k} \pmod{p} \quad (B_{p-k} : \text{Bernoulli number}).$$

To show (7.2), we proceed as follows using Fermat’s little theorem and the Seki–Bernoulli formula (see e.g. [2, Chapter 1]) for sum of powers (assuming  $p$  is large

enough).

$$\begin{aligned} \sum_{0 < m_1 < m_2 < p} \frac{1}{m_1^{k_1} m_2^{k_2}} &\equiv \sum_{m_2=1}^{p-1} \left( \sum_{m_1=1}^{m_2-1} m_1^{p-1-k_1} \right) m_2^{-k_2} \pmod p \\ &\equiv \sum_{m_2=1}^{p-1} \frac{1}{p-k_1} \sum_{i=0}^{p-1-k_1} \binom{p-k_1}{i} B_i \cdot m_2^{p-k_1-i-k_2} \pmod p \\ &\equiv \frac{1}{k_1} \binom{p-k_1}{p-k_1-k_2} B_{p-k_1-k_2} \pmod p \\ &\equiv (-1)^{k_2} \binom{k_1+k_2}{k_2} \frac{B_{p-(k_1+k_2)}}{k_1+k_2} \pmod p. \end{aligned}$$

In the third congruence, we have used  $\sum_{m_2=1}^{p-1} m_2^{p-k_1-i-k_2} \equiv 0 \pmod p$  except for  $i = p - k_1 - k_2$ . This kind of computation, as well as more identities on  $\zeta^{\mathcal{A}}(\mathbf{k})_{(p)}$ , was already appeared in M. Hoffman [10] and J. Zhao [39]. The special case  $\zeta^{\mathcal{A}}(1, k-1)_{(p)}$  can be found in even earlier H. S. Vandiver [34].

As seen above, the naive analogue  $\zeta^{\mathcal{A}}(k)$  of the Riemann zeta value  $\zeta(k)$  is 0. However, there are a good many reasons to believe that the “true” analogue of  $\zeta(k)$  in  $\mathcal{A}$  should be  $Z(k)$ . We shall see the supporting evidences in the sequel, but an intuitive “explanation” (with no rigor) is this:

$$\zeta(k) \underset{\text{Fermat}}{\equiv} \zeta(k - (p - 1)) \underset{\text{Euler}}{=} -\frac{B_{p-k}}{p-k} \equiv Z(k)_{(p)} \pmod p.$$

Since the odd-indexed Bernoulli numbers  $B_n$  are 0 when  $n > 1$ ,  $Z(k) = 0$  for even  $k \geq 2$ . This corresponds via our main conjecture to the fact that  $\zeta(k)$  is in  $\zeta(2)\mathcal{Z}$  when  $k$  is even (Euler). The following question looks very interesting, and seems still open.

**Question.** — *Is  $Z(k) \neq 0$ , or more strongly,  $Z(k) \notin \mathbb{Q}$  if  $k > 1$  is odd?*

### 8. Various identities

In this section, we list several known relations of  $\mathcal{A}$ -finite multiple zeta values. The list is not at all complete and we refer the reader to the references cited in the sequel for further examples.

Perhaps the simplest is the reversal formula

$$\zeta^{\mathcal{A}}(k_r, \dots, k_1) = (-1)^{k_1+\dots+k_r} \zeta^{\mathcal{A}}(k_1, \dots, k_r),$$

which can be seen by replacing  $m_i$  in the definition (7.1) with  $p - m_i$ .

S. Saito and N. Wakabayashi [26] proved an analogue of the classical sum formula:

$$(8.1) \quad \sum_{\substack{k_1+\dots+k_r=k \\ k_r \geq 2}} \zeta^{\mathcal{A}}(k_1, \dots, k_r) = \left( 1 + (-1)^r \binom{k-1}{r-1} \right) Z(k).$$

(They proved a little more general identity.) The restriction  $k_r \geq 2$  may look artificial because there seems to be no reason to exclude the absolutely well-defined values with  $k_r = 1$ .

However, by a theorem of Hoffman [9] and by  $\zeta^{\mathcal{A}}(k) = 0$ , one finds the symmetric sum allowing  $k_r = 1$  as well becomes 0. Recently, S. Seki and Yamamoto look at this sum modulo  $p^2$  and obtain a connection to  $Z(k + 1)$ . It is amusing to remark that the right-hand side of (8.1) is a kind of hybrid of the classical sum formula

$$\sum_{\substack{k_1 + \dots + k_r = k \\ k_r \geq 2}} \zeta(k_1, \dots, k_r) = \zeta(k)$$

and its analogue for the multiple zeta-star values

$$\sum_{\substack{k_1 + \dots + k_r = k \\ k_r \geq 2}} \zeta^*(k_1, \dots, k_r) = \binom{k-1}{r-1} \zeta(k).$$

The analogue (8.1) clearly suggests that  $Z(k)$  should correspond to  $\zeta(k)$ . Analogues of the Le–Murakami relation and the Aoki–Ohno relation are

$$\sum_{\mathbf{k} \in I(k,s)} (-1)^{\text{dep}(\mathbf{k})} \zeta^{\mathcal{A}}(\mathbf{k}) = 2 \binom{k-1}{2s-1} (1 - 2^{1-k}) Z(k)$$

and

$$\sum_{\mathbf{k} \in I(k,s)} \zeta^{\mathcal{A},*}(\mathbf{k}) = 2 \binom{k-1}{2s-1} (1 - 2^{1-k}) Z(k),$$

which were conjectured by the author and were proved by K. Oyama and Saito [16]. Here,  $I(k, s)$  is the set of admissible indices of weight  $k$  and height (number of components greater than 2)  $s$ , and  $\text{dep}(\mathbf{k})$  denotes the depth of an index  $\mathbf{k}$ , and the  $\mathcal{A}$ -multiple zeta-star value  $\zeta^{\mathcal{A},*}(\mathbf{k})$  is defined in the obvious way. The original Aoki–Ohno relation is

$$\sum_{\mathbf{k} \in I(k,s)} \zeta^*(\mathbf{k}) = 2 \binom{k-1}{2s-1} (1 - 2^{1-k}) \zeta(k),$$

and here too the analogy between  $Z(k)$  and  $\zeta(k)$  is obvious.

There is a duality relation due to Hoffman [10]. For a (not necessarily admissible) index  $(k_1, \dots, k_r)$ , its Hoffman’s dual, denoted by  $(k_1, \dots, k_r)^\vee$ , is the index obtained by writing each component  $k_i$  as a sum of 1 and then interchanging commas “,” and plus signs “+”. For example,

$$(n)^\vee = (1 + \dots + 1)^\vee = \underbrace{(1, \dots, 1)}_n, \quad (2, 3)^\vee = (1 + 1, 1 + 1 + 1)^\vee = (1, 1 + 1, 1, 1) = (1, 2, 1, 1).$$

Then, Hoffman’s duality is

$$(8.2) \quad \zeta^{\mathcal{A},*}(k_1, \dots, k_r) = -\zeta^{\mathcal{A},*}((k_1, \dots, k_r)^\vee).$$

This identity is equivalent to the following identity among non-star  $\mathcal{A}$ -finite multiple zeta values (see Hoffman [10, Theorem 4.7]). For any  $\mathbf{k} = (k_1, \dots, k_r)$ , we have

$$\zeta^{\mathcal{A}}(\mathbf{k}) = (-1)^r \sum_{\mathbf{k}' \succeq \mathbf{k}} \zeta^{\mathcal{A}}(\mathbf{k}').$$

Here, for two indices  $\mathbf{k}$  and  $\mathbf{k}'$ , the relation  $\mathbf{k}' \succeq \mathbf{k}$  means the index  $\mathbf{k}$  is obtained by replacing some commas in  $\mathbf{k}' = (k'_1, \dots, k'_s)$  by plus signs, examples being

$$(1, 3, 2, 1) \succeq (1 + 3, 2, 1) = (4, 2, 1), \quad (1, 3, 2, 1) \succeq (1 + 3, 2 + 1) = (4, 3),$$

$$(1, 3, 2, 1) \succeq (1 + 3 + 2 + 1) = (7).$$

Ohno’s relation has also an analogue. Let  $(k_1, \dots, k_r)$  and  $(k'_1, \dots, k'_{r'})$  be admissible indices which are dual with each other in the usual sense. For these and a given integer  $l \geq 0$ , the classical Ohno relation is

$$\sum_{\substack{e_1 + \dots + e_r = l \\ e_i \geq 0}} \zeta(k_1 + e_1, \dots, k_r + e_r) = \sum_{\substack{e'_1 + \dots + e'_{r'} = l \\ e'_i \geq 0}} \zeta(k'_1 + e'_1, \dots, k'_{r'} + e'_{r'}).$$

A  $\zeta^A$ -analogue of this was conjectured by the author and proved by Oyama [23]. Let  $(k_1, \dots, k_r)$  and  $(k^*_1, \dots, k^*_{r^*})$  be indices which are dual with each other in Hoffman’s sense. For these and a given integer  $l \geq 0$ , we have

$$\sum_{\substack{e_1 + \dots + e_r = l \\ e_i \geq 0}} \zeta^A(k_1 + e_1, \dots, k_r + e_r) = \sum_{\substack{e^*_1 + \dots + e^*_{r^*} = l \\ e^*_i \geq 0}} \zeta^A((k^*_1 + e^*_1, \dots, k^*_{r^*} + e^*_{r^*})^\vee).$$

Note that we need to take Hoffman’s dual on the right, so that the case  $l = 0$  becomes trivial. In recent years, many other relations as well as generalizations in various settings are proved and investigated. We refer [6], [12], [14], [15], [20], [21], [22], [25], [27], [29], [28], [31], [32], [40], among others. This is not at all an exhaustive list, and the readers are advised to visit the web page of Hoffman [8] which provides an extensive literature on multiple zeta values and related subjects.

To conclude this section, we present analogues of the double shuffle relation. First, we already mentioned that  $\zeta^A(\mathbf{k})$  satisfies the stuffle product rule:

$$(8.3) \quad \zeta^A(\mathbf{k})\zeta^A(\mathbf{l}) = \zeta^A(\mathbf{k} * \mathbf{l}) \quad (\forall \mathbf{k}, \mathbf{l} \in \mathcal{R}).$$

In particular, when  $\mathbf{l} = (l)$ , this gives linear relations

$$(8.4) \quad \zeta^A(\mathbf{k} * [l]) = 0 \quad (\forall \mathbf{k} \in \mathcal{R}, \forall l \geq 1).$$

As for the shuffle  $\mathfrak{m}$ , we do not have a formula involving products, but we have the following relation.

**Theorem 8.1.** — For any  $\mathbf{k}$  and  $\mathbf{l}$  in  $\mathcal{R}$ ,

$$(8.5) \quad \zeta^A(\mathbf{k} \mathfrak{m} \mathbf{l}) = (-1)^{|\mathbf{l}|} \zeta^A(\mathbf{k}, \overleftarrow{\mathbf{l}}),$$

where  $|\mathbf{l}|$ ,  $\overleftarrow{\mathbf{l}}$  are respectively the weight and the reversal of  $\mathbf{l}$ , and  $(\mathbf{k}, \overleftarrow{\mathbf{l}})$  on the right is the concatenation of  $\mathbf{k}$  and  $\overleftarrow{\mathbf{l}}$ .

*Proof.* — This is easily proved by using the shuffle product of the multiple polylogarithm

$$\text{Li}_{\mathbf{k}}(x) = \text{Li}_{k_1, \dots, k_r}(z) = \sum_{0 < m_1 < \dots < m_r} \frac{z^{m_r}}{m_1^{k_1} \dots m_r^{k_r}}.$$

As is well known, this satisfies

$$\text{Li}_{\mathbf{k}}(z) \text{Li}_{\mathbf{l}}(z) = \text{Li}_{\mathbf{k}\mathfrak{m}\mathbf{l}}(z).$$

Here, the right-hand side is the sum  $\sum_{\mathbf{m}} \text{Li}_{\mathbf{m}}(z)$  where  $\mathbf{k} \boxplus \mathbf{l} = \sum_{\mathbf{m}} [\mathbf{m}]$  in  $\mathcal{R}_{\boxplus}$ . Since

$$\zeta_p(\mathbf{k}) = \sum_{0 < m_1 < \dots < m_r < p} \frac{1}{m_1^{k_1} \dots m_r^{k_r}} = \sum_{0 < m < p} (\text{coefficient of } z^m \text{ in } \text{Li}_{\mathbf{k}}(z)),$$

we can compute

$$\begin{aligned} \zeta_p(\mathbf{k} \boxplus \mathbf{l}) &= \sum_{0 < m < p} (\text{coefficient of } z^m \text{ in } \text{Li}_{\mathbf{k} \boxplus \mathbf{l}}(z)) \\ &= \sum_{\substack{0 < i, j < p \\ 0 < i+j < p}} (\text{coefficient of } z^i \text{ in } \text{Li}_{\mathbf{k}}(z)) \cdot (\text{coefficient of } z^j \text{ in } \text{Li}_{\mathbf{l}}(z)) \\ &= \sum_{0 < i, j, i+j < p} \left( \sum_{0 < m_1 < \dots < m_{r-1} < i} \frac{1}{m_1^{k_1} \dots m_{r-1}^{k_{r-1}} i^{k_r}} \right) \left( \sum_{0 < n_1 < \dots < n_{s-1} < j} \frac{1}{n_1^{l_1} \dots n_{s-1}^{l_{s-1}} j^{l_s}} \right) \\ &\equiv \sum_{0 < i, j, i+j < p} \left( \left( \sum_{0 < m_1 < \dots < m_{r-1} < i} \frac{1}{m_1^{k_1} \dots m_{r-1}^{k_{r-1}} i^{k_r}} \right) \right. \\ &\quad \left. \times \left( \sum_{p-j < p-n_{s-1} < \dots < p-n_1 < p} \frac{(-1)^{|\mathbf{l}|}}{(p-n_1)^{l_1} \dots (p-n_{s-1})^{l_{s-1}} (p-j)^{l_s}} \right) \right) \pmod p \\ &\equiv \sum_{0 < m_1 < \dots < m_{r-1} < i < j < n_{s-1} < \dots < n_1 < p} \frac{(-1)^{|\mathbf{l}|}}{m_1^{k_1} \dots m_{r-1}^{k_{r-1}} i^{k_r} j^{n_s} n_{s-1}^{l_{s-1}} \dots n_1^{l_1}} \pmod p \\ &= (-1)^{|\mathbf{l}|} \zeta^{\mathcal{A}}(\mathbf{k}, \overleftarrow{\mathbf{l}})_{(p)}. \end{aligned}$$

□

We propose the following conjecture based on the numerical evidence up to weight 18 (thanks to T. Machide). But the word “conjecture” may be too strong because a theoretical support is still missing.

**Conjecture 8.2.** — *Any relations in  $\mathcal{Z}_{\mathcal{A}}$  of finite multiple zeta values can be deduced from (8.3) and (8.5). Moreover, any linear relations are consequences of (8.4) and (8.5).*

### 9. Symmetric multiple zeta values

Consider the following sums for any index  $\mathbf{k} = (k_1, \dots, k_r) \in \mathcal{R}$ .

$$\begin{aligned} \zeta^{\mathcal{S},*}(\mathbf{k}) &:= \sum_{i=0}^r (-1)^{k_{i+1} + \dots + k_r} \zeta_*(k_1, \dots, k_i; T) \zeta_*(k_r, \dots, k_{i+1}; T), \\ \zeta^{\mathcal{S},\boxplus}(\mathbf{k}) &:= \sum_{i=0}^r (-1)^{k_{i+1} + \dots + k_r} \zeta_{\boxplus}(k_1, \dots, k_i; T) \zeta_{\boxplus}(k_r, \dots, k_{i+1}; T). \end{aligned}$$

Here,  $\zeta_*$  and  $\zeta_{\boxplus}$  are regularized polynomials introduced in Section 4. A priori, the right-hand sides depend on  $T$ , but actually they do not.

**Proposition 9.1.** —

- (1) Both  $\zeta^{\mathcal{S},*}(\mathbf{k})$  and  $\zeta^{\mathcal{S},\boxplus}(\mathbf{k})$  are in  $\mathcal{Z}_k$  ( $k = \text{weight of } \mathbf{k}$ ), independent of  $T$ .

(2) We have  $\zeta^{\mathcal{S},*}(\mathbf{k}) - \zeta^{\mathcal{S},\text{III}}(\mathbf{k}) \in \zeta(2)\mathcal{Z}$ .

We can prove these by using the identity

$$\sum_{s=0}^{\infty} \zeta_{\bullet}(\mathbf{k}, \underbrace{1, \dots, 1}_s; T)x^s = e^{Tx} \sum_{i=0}^{\infty} \zeta_{\bullet}(\mathbf{k}, \underbrace{1, \dots, 1}_i; 0)x^i \quad (\bullet = * \text{ or III})$$

for any admissible  $\mathbf{k}$  ([11, Proposition 10]), and the fundamental relation (4.2). An alternative way to prove (1)) is to work in  $\mathcal{R}$  to show for instance

$$\sum_{i=0}^r (-1)^{k_{i+1} + \dots + k_r} [k_1, \dots, k_i] * [k_r, \dots, k_{i+1}] \in \mathcal{R}_*^0$$

directly. We refer [18] for details.

Where these strange-looking sums come from? An answer is the following fact:

$$(9.1) \quad \zeta^{\mathcal{S},*}(k_1, \dots, k_r) = \lim_{M \rightarrow \infty} \sum_{\substack{m_1 \prec \dots \prec m_r \\ 0 < |m_i| < M}} \frac{1}{m_1^{k_1} \dots m_r^{k_r}},$$

where the order  $\prec$  on non-zero integers is defined by

$$1 \prec 2 \prec 3 \prec \dots \prec (\infty = -\infty) \prec \dots \prec -3 \prec -2 \prec -1.$$

This order was suggested by M. Kontsevich to Zagier in a private communication indicating the sum  $\sum_{0 < m_1 < m_2 < p}$  to define  $\zeta^A(k_1, k_2)$  becomes  $\sum_{0 < m_1 < m_2 < 0}$  modulo  $p!$  If we divide the sum on the right of (9.1) according as  $0 < m_1 < \dots < m_i$  and  $m_{i+1} < \dots < m_r < 0$  for  $i = 0, \dots, r$ , we are naturally led to the sum in the definition of  $\zeta^{\mathcal{S},*}(\mathbf{k})$ . The details will be discussed in [18]. Assuming (9.1), we immediately see the following proposition.

**Proposition 9.2.** — For any  $\mathbf{k}$  and  $\mathbf{l}$  in  $\mathcal{R}$ , we have

$$(9.2) \quad \zeta^{\mathcal{S},*}(\mathbf{k})\zeta^{\mathcal{S},*}(\mathbf{l}) = \zeta^{\mathcal{S},*}(\mathbf{k} * \mathbf{l}).$$

Again an alternative way is to work in  $\mathcal{R}$ , though the computation becomes tedious. In view of Proposition 9.1, we are naturally led to define an element  $\zeta^{\mathcal{S}}(k_1, \dots, k_r)$  in the quotient algebra  $\mathcal{Z}/\zeta(2)\mathcal{Z}$  of  $\mathcal{Z}$  modulo the ideal generated by  $\zeta(2)$  (or  $\pi^2$ ).

**Definition 9.3.** — For any  $\mathbf{k} \in \mathcal{R}$ , define

$$\zeta^{\mathcal{S}}(\mathbf{k}) := \zeta^{\mathcal{S},\bullet}(\mathbf{k}) \bmod \zeta(2) \in \mathcal{Z}/\zeta(2)\mathcal{Z} \quad (\bullet = * \text{ or III}).$$

We give examples in depths 1 and 2.

**Example 9.4.** —

(1) Depth 1 case: For  $k \geq 1$ ,

$$\zeta^{\mathcal{S},*}(k) = (-1)^k \zeta^*(k) + \zeta^*(k) = \begin{cases} 2\zeta(k) \equiv 0 \pmod{\zeta(2)} & k: \text{ even,} \\ 0 & k: \text{ odd.} \end{cases}$$

Hence  $\zeta^{\mathcal{S}}(k) = 0$  in  $\mathcal{Z}_{\mathbb{R}}/\zeta(2)\mathcal{Z}_{\mathbb{R}}$ . Recall  $\zeta^A(k) = 0$ .

(2) Depth 2 case:

$$\begin{aligned} &\zeta^{\mathcal{S},*}(k_1, k_2) \\ &= (-1)^{k_1+k_2} \zeta_*(k_2, k_1; T) + (-1)^{k_2} \zeta_*(k_1; T) \zeta_*(k_2; T) + \zeta_*(k_1, k_2; T) \\ &\equiv_{\text{mod } \zeta(2)} \begin{cases} 0 & k_1 + k_2: \text{ even,} \\ \zeta_*(k_1, k_2; T) - \zeta_*(k_2, k_1; T) \equiv (-1)^{k_2} \binom{k_1 + k_2}{k_1} \zeta(k_1 + k_2) & k_1 + k_2: \text{ odd.} \end{cases} \end{aligned}$$

Here we used a formula in [38, Proposition 7] to compute the odd weight case (even case is easy by Euler). Since  $\zeta(k_1 + k_2) = 0$  in  $\mathcal{Z}/\zeta(2)\mathcal{Z}$  when  $k_1 + k_2$  is even, we may uniformly write

$$\zeta^{\mathcal{S}}(k_1, k_2) = (-1)^{k_2} \binom{k_1 + k_2}{k_1} \zeta(k_1 + k_2) \pmod{\zeta(2)} \in \mathcal{Z}/\zeta(2)\mathcal{Z}.$$

Compare this with (7.2). Under the correspondence  $\zeta(k) \leftrightarrow Z(k)$ , the right-hand sides are exactly the same.

Now our main conjecture is stated as

**Conjecture 9.5.** — *There is a  $\mathbb{Q}$ -algebra isomorphism between  $\mathcal{Z}_A$  and  $\mathcal{Z}/\zeta(2)\mathcal{Z}$  under which  $\zeta^A(\mathbf{k})$  corresponds to  $\zeta^{\mathcal{S}}(\mathbf{k})$  ( $\forall \mathbf{k} \in \mathcal{R}$ ):*

$$\begin{array}{ccc} \mathcal{Z}_A & \stackrel{?}{\simeq} & \mathcal{Z}/\zeta(2)\mathcal{Z} \\ \Downarrow & & \Downarrow \\ \zeta^A(\mathbf{k}) & \longleftrightarrow & \zeta^{\mathcal{S}}(\mathbf{k}). \end{array}$$

According to this conjecture, any relations among  $\zeta^A(\mathbf{k})$  should hold in exactly the same form in  $\mathcal{Z}/\zeta(2)\mathcal{Z}$  by replacing  $\zeta^A$  with  $\zeta^{\mathcal{S}}$  and vice versa. Many relations are in fact proved both for  $\zeta^A$  and  $\zeta^{\mathcal{S}}$  in the same forms. Notably, the shuffle relation (8.5) holds also for  $\zeta^{\mathcal{S}}$ .

**Theorem 9.6.** — *For any  $\mathbf{k}$  and  $\mathbf{l}$  in  $\mathcal{R}$ , we have the relation*

$$(9.3) \quad \zeta^{\mathcal{S}}(\mathbf{k} \text{ III } \mathbf{l}) = (-1)^{|\mathbf{l}|} \zeta^{\mathcal{S}}(\mathbf{k}, \overleftarrow{\mathbf{l}})$$

in  $\mathcal{Z}/\zeta(2)\mathcal{Z}$ .

In fact, we can prove the exact identity

$$\zeta^{\mathcal{S},\text{III}}(\mathbf{k} \text{ III } \mathbf{l}) = (-1)^{|\mathbf{l}|} \zeta^{\mathcal{S},\text{III}}(\mathbf{k}, \overleftarrow{\mathbf{l}})$$

in  $\mathcal{Z}$ , without taking modulo  $\zeta(2)$ . If we let  $\mathbf{k} = (k_1, \dots, k_i)$  and  $\mathbf{l} = (k_r, \dots, k_{i+1})$ , this identity becomes

$$(9.4) \quad \zeta^{\mathcal{S},\text{III}}(k_1, \dots, k_r) = (-1)^{k_{i+1} + \dots + k_r} \zeta^{\mathcal{S},\text{III}}([k_1, \dots, k_i] \text{ III } [k_r, \dots, k_{i+1}]).$$

We may prove this on the level of indices. Let  $\mathcal{R}^{(r)}$  be the  $\mathbb{Q}$ -span of indices of depth  $r$ . Define a linear map  $S_i^{(r)}$  from  $\mathcal{R}^{(r)}$  to itself by

$$S_i^{(r)}([k_1, \dots, k_r]) := (-1)^{k_{i+1} + \dots + k_r} [k_1, \dots, k_i] \text{ III } [k_r, \dots, k_{i+1}] \quad (0 \leq i \leq r),$$

and set  $S^{(r)} := \sum_{i=0}^r S_i^{(r)}$ . Then we have  $\zeta^{\mathcal{S},\text{III}}(\mathbf{k}) = \zeta_{\text{III}}(S^{(r)}(\mathbf{k}); T)$ , and the identity (9.4) follows from the following.



**Proposition 9.7.** — *We have*

$$S^{(r)} \circ S_i^{(r)} = S^{(r)}.$$

To prove this, we use the generating function

$$F(x_1, \dots, x_r) := \sum_{k_1, \dots, k_r \geq 1} [k_1, \dots, k_r] x_1^{k_1-1} \dots x_r^{k_r-1} \in \mathcal{R}_{\text{III}}[x_1, \dots, x_r]$$

and reduces the identity, by a similar consideration developed in [11, Section 8], to the following identity in the group ring  $\mathbb{Z}[\mathfrak{S}_{r+1}]$  of the symmetric group: Let

$$U_i^{(r)} := \{\sigma \in \mathfrak{S}_{r+1} \mid \sigma(1) < \dots < \sigma(i+1) > \dots > \sigma(r+1)\}$$

be the set of “unimodal” elements and set

$$u_i^{(r)} = \sum_{\sigma \in U_i^{(r)}} \sigma$$

and

$$u_{\text{alt}}^{(r)} = \sum_{i=0}^r (-1)^{r-i} u_i^{(r)}.$$

Then we have the identity

$$(9.5) \quad u_{\text{alt}}^{(r)} \cdot (-1)^{r-i} u_i^{(r)} = u_{\text{alt}}^{(r)}$$

in  $\mathbb{Z}[\mathfrak{S}_{r+1}]$ . It turns out that this is equivalent to an identity of Specht [30, (24)] in “descent algebra” (see also [24, Lemma 8.18]), and the proof is completed. See [18] for more details.

**Remark 9.8.** —

- (1) S. Yasuda supplied a proof of the identity (9.5) before the author learned that it was actually a classical identity.
- (2) D. Jarrosay proved (9.3) by using Drinfeld’s associator [13]. Recently, M. Hirose [7] defined an object  $\zeta^{RS}(\mathbf{k})$  in  $\mathbb{C}$  which “lifts”  $\zeta^S(\mathbf{k})$  by a simple integral. This new quantity satisfies the shuffle product formula as an immediate consequence from the definition as an integral, and by taking the real part of the formula, our (9.3) follows. Arguably this is the most natural proof of (9.3). The  $\zeta^{RS}(\mathbf{k})$  also appeared in a recent work of H. Bachmann, Y. Takeyama, and K. Tasaka [3], where they discovered a unified way to obtain both  $\zeta^A(\mathbf{k})$  and  $\zeta^S(\mathbf{k})$  from a single object, a  $q$ -multiple zeta value, by specializations. This may shed light on our Conjecture 9.5.

We may pose the  $\zeta^S$ -version of Conjecture 8.2. At least, to try to deduce various identities from (9.2) and (9.3) may be a good challenge.

Finally, we remark that the conjecture implies  $\zeta^S(\mathbf{k})$ ’s generate  $\mathcal{Z}/\zeta(2)\mathcal{Z}$ . But what’s more, Yasuda proved in [37] that either of  $\zeta^{S,*}(\mathbf{k})$ ’s or  $\zeta^{S,\text{III}}(\mathbf{k})$ ’s already generate the whole  $\mathcal{Z}$ .

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