FINITE MULTIPLE ZETA VALUES

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Contents

Introduction

The title of this paper refers to two very different "finite" versions of the classical multiple zeta values[1]

$$\zeta(\mathbf{k}) \;=\; \zeta(k_1,\dots,k_r) \;=\; \sum_{0<n_1<\cdots<n_r} \frac{1}{n_1^{k_1}\cdots n_r^{k_r}} \quad \in \mathbb{R} \qquad (k_1,\dots,k_r\in\mathbb{N}), \tag{1}$$

[1] Some authors use the opposite convention, with $n_1 > \cdots > n_r > 0$ in the summation. As we will see in a moment, in the finite case this becomes almost irrelevant since the two numbers are the same up to a sign.

which are very interesting real numbers if $k_r \geq 2$ ("$\mathbf{k}$ admissible") but are infinite if $k_r = 1$. The first of these is the element $\zeta_{\mathcal{A}}(\mathbf{k})$ of the "poor man's adele ring"

$$\mathcal{A} \;:=\; \prod_{p \text{ prime}} \mathbb{Z}/p\mathbb{Z} \Big/ \bigoplus_{p \text{ prime}} \mathbb{Z}/p\mathbb{Z} \tag{2}$$

defined by $\zeta_{\mathcal{A}}(\mathbf{k}) \;=\; \bigl(\zeta_p(\mathbf{k}) \mod p\bigr)_{p \text{ prime}}$, where $\zeta_p(\mathbf{k})$ for each prime p is given by

$$\zeta_p(k_1,\dots,k_r) \;=\; \sum_{0<n_1<\cdots<n_r<p} \frac{1}{n_1^{k_1}\cdots n_r^{k_r}}\,. \tag{3}$$

The other is the *symmetric multiple zeta value* or *finite real multiple zeta value* defined by

$$\zeta_S(k_1,\dots,k_r) \;=\; \sum_{s=0}^{r}(-1)^{k_{s+1}+\cdots+k_r}\zeta(k_1,\dots,k_s)\zeta(k_r,\dots,k_{s+1}) \mod \pi^2\,. \tag{4}$$

This is obviously finite if all k_s are ≥ 2, but turns out also to be finite if the k_s are arbitrary positive integers and any divergent multiple zeta values appearing in the right-hand side of (4) are replaced by their regularized values as defined in §7. Actually, there are two versions depending whether the multiple zeta values in (4) are replaced by their $*$ or $ш$ regularizations, where $*$ and $ш$ are the well-known series and integral shuffle products satisfying $\zeta(\mathbf{k})\zeta(\mathbf{l}) = \zeta(\mathbf{k}*\mathbf{l}) = \zeta(\mathbf{k}ш\mathbf{l})$ if both $\mathbf{k}$ and $\mathbf{l}$ are admissible (their definitions will be recalled in §7), but the two versions are congruent modulo the principal ideal of $\mathfrak{Z}$ (the ring of real multiple zeta values) generated by π^2, so that we have a well-defined element $\zeta_S(\mathbf{k}) \in \mathfrak{Z}/(\pi^2)$ for every tuple $\mathbf{k}$, admissible or not. Our main discovery, based on extensive computer calculations and a number of theoretical results, is the following conjectural isomorphism.

Main Conjecture. *There exists an isomorphism*

$$\begin{array}{ccc} \mathfrak{Z}_{\mathcal{A}} & \cong & \mathfrak{Z}^{\mathrm{red}} \;:=\; \mathfrak{Z}/(\pi^2) \\ \zeta_{\mathcal{A}}(\mathbf{k}) & \longleftrightarrow & \zeta_S(\mathbf{k}), \end{array} \tag{5}$$

where $\mathfrak{Z}_{\mathcal{A}}$ is the subring of $\mathcal{A}$ spanned by the $\zeta_{\mathcal{A}}(\mathbf{k})$. This isomorphism is compatible with both the grading by weight and the filtration by depth of the two rings, where the weight of both $\zeta_{\mathcal{A}}(\mathbf{k})$ and $\zeta_S(\mathbf{k})$ for $\mathbf{k} = (k_1,\dots,k_r)$ is given by $|\mathbf{k}| = k_1+\cdots+k_r$, while the depth filtration on $\mathfrak{Z}_{\mathcal{A}}$ is defined by the depth of $\zeta_{\mathcal{A}}(\mathbf{k})$ being $\leq r-1$.

In particular, this conjecture says that the depth of $\zeta_S(\mathbf{k})$ is $\leq r-1$, i.e. $\zeta_S(k_1,\dots,k_r)$ modulo π^2 is always a rational linear combination of MZVs $\zeta(k'_1,\dots,k'_{r'})$ with $r' < r$.

Note that, although (3) is the natural $\mathbb{F}_p$-analogue of $\zeta(\mathbf{k})$ and $\zeta_{\mathcal{A}}(\mathbf{k})$ therefore its natural $\mathcal{A}$-analogue, the number $\zeta_{\mathcal{A}}(\mathbf{k})$ is *not* the image of $\zeta(\mathbf{k})$ under the conjectural isomorphism (5). For instance, if $r = 1$, $\mathbf{k} = (k)$ the finite MZV $\zeta_{\mathcal{A}}(k)$ always vanishes, whereas the real MZV $\zeta(k)$ for k odd is conjectured not to belong to $\pi^2\mathfrak{Z}$. We refer to §5 for more discussion of this point.

If the isomorphism (5) holds, then the well-known conjecture that $\mathfrak{Z}$ is the direct sum $\oplus\mathfrak{Z}_k$ (where $\mathfrak{Z}_k$ is the $\mathbb{Q}$-space spanned by all $\zeta(\mathbf{k})$ with weight $|\mathbf{k}| = k_1+\cdots+k_r$ equal to k) and that the dimension of $\mathfrak{Z}_k$ is equal to the number d_k defined by the generating function $\sum d_k x^k = \frac{1}{1-x^2-x^3}$, corresponds to the conjectural formula

$$\sum_{k=0}^{\infty} \dim_{\mathbb{Q}}\bigl(\mathfrak{Z}_{\mathcal{A},k}\bigr)\,x^k \;\overset{?}{=}\; \frac{1-x^2}{1-x^2-x^3} \;=\; 1+\sum_{k=3}^{\infty} d_{k-3}\,x^k\,, \tag{6}$$

where $\mathfrak{Z}_{\mathcal{A},k}$ denotes the $\mathbb{Q}$-span of the $\zeta_{\mathcal{A}}(\mathbf{k})$ of weight k. This has been checked numerically (and the upper bound checked theoretically) up to about weight 20. For instance, for $k = 11$ we find to high precision in $\mathcal{A}$, and then prove rigorously, that the space $\mathfrak{Z}_{\mathcal{A},k}$ is spanned by the four numbers $\zeta_{\mathcal{A}}(1,10)$, $\zeta_{\mathcal{A}}(1,1,1,8)$, $\zeta_{\mathcal{A}}(1,1,2,7)$ and $\zeta_{\mathcal{A}}(1,1,5,4)$, a typical identity being

$$\zeta_{\mathcal{A}}(2,3,1,2,3) = \frac{61793}{1728}\zeta_{\mathcal{A}}(1,10) - \frac{125}{3}\zeta_{\mathcal{A}}(1,1,1,8) - \frac{265}{36}\zeta_{\mathcal{A}}(1,1,2,7) + \frac{53}{18}\zeta_{\mathcal{A}}(1,1,5,4), \quad (7)$$

and the conjectural isomorphism (5) is illustrated by the fact that the same relation holds numerically for the corresponding symmetric multiple zeta values, up to an element of the 5-dimensional $\mathbb{Q}$-vector space $\pi^2\mathfrak{Z}_9$.

We will discuss the $\mathcal{A}$-multiple zeta values (henceforth often "$\mathcal{A}$MZVs") in Part I of the paper (§§1–6), and the symmetric multiple zeta values (SMZVs) and their conjectural relationship to $\mathcal{A}$MZVs in Part II (§§7–9). In more detail, the contents of the various sections are as follows. In §1 we discuss the properties of the ring $\mathcal{A}$ and describe a number of its interesting elements, as well as explaining how to do numerical computations to high accuracy in this ring. One of the families of special elements that we define, the "harmonic moment sums" or "Sun sums," is then discussed in detail in §2. These sums turn out to be linear combinations of $\mathcal{A}$MZVs, to which the remaining sections are devoted. In §3 we list a number of known or conjectured special identities among $\mathcal{A}$MZVs (many of them found or proved by other authors; this section has partially the character of a survey), including an interesting relation to cusp forms on the full modular group $\mathrm{SL}_2(\mathbb{Z})$. In §4, we introduce "multiple Seki-Bernoulli sums," which span the same space as $\mathcal{A}$MZVs and will be used to construct conjectural "true" multiple zeta values (meaning the elements that correspond to the real MZVs $\zeta(\mathbf{k}) \in \mathfrak{Z}^{\mathrm{red}}$ under the isomorphism (5)) in $\mathcal{A}$, which is the subject of §5. In §6 we show that the subspace $\mathfrak{Z}_{\mathcal{A}}$ of $\mathcal{A}$ spanned by all $\mathcal{A}$MZVs is a ring having a depth filtration similar to the one for classical MZVs, but with the depth now one less than the length of the argument, and prove a shuffle relation that can be considered as the $\mathcal{A}$MZV-analogue of the so-called double shuffle relations in the classical case. After recalling shuffle relations and regularizations of classical MZVs in §7, we define and study the symmetric multiple zeta values in §8. In particular, we prove the shuffle relation corresponding to the one for $\mathcal{A}$MZVs under the main conjecture. In the final §9, we present several conjectural isomorphisms among the spaces of $\mathcal{A}$MZVs, SMZVs, and some quotient algebras of formal space of indices modulo various ideals.

Remark 1. In the interests of full disclosure, we should perhaps say here that it is not known that even a single one of the $\mathcal{A}$MZVs $\zeta_{\mathcal{A}}(\mathbf{k})$ studied in this paper is non-zero! (We of course know that many of them have non-vanishing p-components for a large number of primes p, but that does not prevent them from vanishing in $\mathcal{A}$.) This is of course embarrassing, but a little less so if we recall that even for the much more intensively studied classical multiple zeta values $\zeta(\mathbf{k})$, there is not a single one that is known not to be a rational multiple of the appropriate power of π.

Remark 2. The work described in this paper was begun in 2012, but for various reasons was very slow to get written up. The conjectures and results it contains were widely disseminated and are referred to and extended in many papers, several of which are listed in the bibliography, and our main conjecture can now even be found in a Japanese manga ([27], p. 115).

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Part I: $\mathcal{A}$-multiple zeta values and their variants

Part I of this paper is concerned with the ring $\mathcal{A}$ of "poor man's adeles". In the first section we describe some of its interesting elements, and also briefly indicate how to do numerical computations in it. The other sections concentrate on the finite MZVs, beginning with Sun's "harmonic moment sums," which are special cases, discuss a number of proved or conjectural special identities among finite MZVs, and discuss an alternative approach using Bernoulli numbers.

1. The ring $\mathcal{A}$ and some of its special elements

In this preliminary section we describe a number of interesting special elements of the ring $\mathcal{A}$. Three of them (those defined in Examples **2.**, **5.** and **7.** below) will then be treated in more detail in the remainder of the paper.

Example 1: Rational numbers. If x is a rational number, then for every prime p not dividing the denominator of x one can consider the image of x in $\mathbb{Z}/p\mathbb{Z}$. This defines an element, also denoted x, in $\mathcal{A}$. (Here and from now on, when defining an element of $\mathcal{A}$, we simply ignore components that are not well-defined, since the definition of $\mathcal{A}$ allows us to omit finitely many components.) This gives a canonical and injective ring homomorphism $\mathbb{Q} \hookrightarrow \mathcal{A}$ and makes $\mathcal{A}$ into a $\mathbb{Q}$-algebra. Note that we can also write $\mathcal{A} = \mathcal{A}_0 \otimes_{\mathbb{Z}} \mathbb{Q} = \mathcal{A}_0/(\mathcal{A}_0)_{\mathrm{tors}}$, where $\mathcal{A}_0 = \prod_p \mathbb{Z}/p\mathbb{Z}$. We mention that the ring $\mathcal{A}$ is also a quotient of the adele ring of $\mathbb{Q}$ in an obvious way.

Example 2: Harmonic moment sums. These sums, which the second author learned about from a talk given by Zhi-Wei Sun in Taiwan in 2010, were the starting point for the current paper. For $i \in \mathbb{Z}$ and $j \in \mathbb{Z}_{\geq 0}$, we define the *harmonic moment sum* or *Sun sum* $V(i,j) \in \mathcal{A}$ by

$$V(i,j)_{(p)} \;=\; \sum_{n=1}^{p-1} n^i H_n^j \pmod{p}\,, \tag{8}$$

where $H_n = 1 + \frac{1}{2} + \cdots + \frac{1}{n}$ denotes the nth harmonic sum. These sums were introduced by Sun, who discovered numerically that, for example, $V(2,2) = -4/9$. (This formula, still conjectural at the time of the lecture just mentioned, is proved in [45], but has been rewritten in our notation: Sun does not consider the ring $\mathcal{A}$, but rather studies each component $V(i,j)_{(p)}$ separately.) We will consider these numbers in detail in §2, where we will show that many of the numbers $V(i,j)$ belong to the subring $\mathbb{Q}$ of $\mathcal{A}$, typical examples being

$$V(6,2) \;=\; \frac{76}{2205}\,, \qquad V(8,3) \;=\; -\frac{17588}{165375}\,, \qquad V(5,4) \;=\; \frac{59}{2250}\,. \tag{9}$$

More generally, we will see that the values of $V(i,j)$ with j fixed and i running over all positive integers belong to some finite-dimensional $\mathbb{Q}$-vector subspace of $\mathcal{A}$ containing $\mathbb{Q}$ (for instance, all of the numbers $V(i,4)$ with $i \geq 0$ belong to the 2-dimensional[2] subspace of $\mathcal{A}$ spanned by 1 and the number $Z_{\mathcal{A}}(3)$ defined in Example 5 below), while the numbers $V(i,j)$ for $i < 0$ are homogeneous elements of the ring of finite multiple zeta values defined in Example 7 below.

[2]More properly, "at most 2-dimensional," since one does not know the linear independence of 1 and $Z_{\mathcal{A}}(3)$.

Example 3: Fermat quotients. If x is a rational number, then Fermat's "little" theorem tells us that $x^{p-1} \equiv 1 \pmod{p}$ (if x is prime to p), so that we can consider the quotient

$$L(x)_{(p)} \;=\; \frac{x^{p-1}-1}{p} \pmod{p} \quad\in\quad \mathbb{Z}/p\mathbb{Z}\,,$$

defining an element $L(x) = (L(x)_{(p)})_p \in \mathcal{A}$. This defines a map $L : \mathbb{Q}^\times \to \mathcal{A}$. It is easy to verify that $L(xy) = L(x) + L(y)$ for all $x, y \in \mathbb{Q}^\times$, so that the Fermat quotient map L can be considered as the $\mathcal{A}$-version of the logarithm map.

Another natural choice for an $\mathcal{A}$-logarithm would be the function $L_1 : \mathbb{Q} \to \mathcal{A}$ defined by

$$L_1(x)_{(p)} \;=\; -\sum_{0<n<p} \frac{(1-x)^n}{n}\,.$$

However, this function does not behave well under multiplication. Instead, we have the nice formula

$$L_1(x) \;=\; xL(x) - (x-1)L(x-1)\,,$$

whose easy proof is left to the reader. (Hint: expand $(x^p - (x-1)^p - 1)/p$ by the binomial theorem.)

Example 4: Wilson quotients and the $\mathcal{A}$-analogue of Euler's constant. Similarly, Wilson's theorem tells us that we have a congruence $(p-1)! \equiv -1 \pmod{p}$ for all primes p, so that we can consider the quotient

$$\gamma_{(p)} \;=\; \frac{(p-1)!\,+1}{p} \bmod p \quad\in\quad \mathbb{Z}/p\mathbb{Z}\,, \tag{10}$$

defining an element $\gamma_{\mathcal{A}} = (\gamma_{(p)})_p$ of $\mathcal{A}$. According to a private communication of Maxim Kontsevich, who has considered the ring $\mathcal{A}$ in a different context [28],[3] this number should be considered as the $\mathcal{A}$-analogue of Euler's constant $\gamma = \lim\bigl(H_n - \log n\bigr)$, whence the notation. We refer to [23] for further discussion.

Example 5: Zeta values. Our next example involves Bernoulli numbers. Define $Z_{\mathcal{A}}(3) \in \mathcal{A}$ by

$$Z_{\mathcal{A}}(3)_{(p)} \;=\; \frac{B_{p-3}}{3} \bmod p\,,$$

where B_n is the nth Bernoulli number. We think of this number as the $\mathcal{A}$-analogue of the Riemann zeta value $\zeta(3) = 1.2020569\cdots \in \mathbb{R}$. The motivation for this interpretation is that $\zeta(1-n) = -B_n/n$ for all $n > 1$ by Euler's formula, and that the numbers $B_n/n \bmod p$ ($n \not\equiv 0 \pmod{p-1}$) are periodic in n with period $p-1$, so that extrapolating backwards we can think of $Z_{\mathcal{A}}(3)_{(p)}$ as the mod p reduction of $\zeta(3) = \zeta(1-(-2))$ ("$\equiv$"$\zeta(1-(p-3)) \pmod{p}$).

More generally, we define $Z_{\mathcal{A}}(k) \in \mathcal{A}$ for $k > 1$ by

$$Z_{\mathcal{A}}(k)_{(p)} \;=\; \frac{B_{p-k}}{k} \bmod p\,, \tag{11}$$

and consider this as the $\mathcal{A}$-version of $\zeta(k)$. Notice that $Z_{\mathcal{A}}(k)$ vanishes identically for $k = 2, 4, \ldots$ because $B_n = 0$ for $n > 1$ odd. In view of Euler's formula $\zeta(k) \in \mathbb{Q}\,\pi^k$ for even k, this can be interpreted as the statement that the $\mathcal{A}$-analogue of π, or at least of π^2, vanishes, a statement that is intuitively unsurprising because the $\mathcal{A}$-analogue $L : \mathbb{Q}^\times/\{\pm 1\} \to \mathcal{A}$ of the logarithm

[3]However, the appearance of the ring $\mathcal{A}$ in the literature goes back at least, as far as the authors are aware, to 1968. See Theorem B in [3]

map as defined above is presumably injective, and this suggests that the correct $\mathcal{A}$-analogue of $2\pi i$ should be 0. It is overwhelmingly likely, and would follow immediately from the widely believed statement that there are infinitely many regular primes, that $Z_{\mathcal{A}}(k) \neq 0$ for every odd $k \geq 3$, but this is currently not known for a single value. It can happen that individual values of $Z_{\mathcal{A}}(k)_{(p)}$ vanish, but the expectation is that for each fixed value of k this happens only for a very thin set of primes p (roughly $\log\log x$ primes less than x as $x \to \infty$), and certainly not for all sufficiently large primes. In particular, in the case $k = 3$ the vanishing of $Z_{\mathcal{A}}(3)_{(p)}$, i.e., the divisibility of B_{p-3} by p, is known to be equivalent to the strengthening of Wolstenholme's congruence $\binom{2p}{p} \equiv 2 \pmod{p^3}$ to $\binom{2p}{p} \equiv 2 \pmod{p^4}$, a congruence that occasionally holds but is certainly most unlikely to be true for all large p. (The only two known occurrences, and the only ones less than 12000000, are for $p = 16843$ and $p = 2124679$. See [27], p. 107.)

We remark that the idea leading to the definition (11) can be extended to give a definition of at least double and triple zeta values in the ring $\mathcal{A}$ that are *not* just the $\mathcal{A}$-multiple zeta values with $r = 2$ or 3 introduced in Example 7 below and studied in this paper. These new values, whose definition is completely heuristic, agree numerically with the "right" things according to our main conjecture, and will be discussed in detail in §5.

Example 6: Weighted sums of Bell numbers. The Bell numbers B_n (not to be confused with the Bernoulli numbers with the same notation) are the numbers 1, 1, 2, 5, 15, 52, … given by the generating function $\sum \mathsf{B}_n x^n/n! = \exp(e^x - 1)$ or by the "closed" formula $\sum k^n/k! = \mathsf{B}_n\, e$. It was discovered experimentally by Zhi-Wei Sun, and proved by him and the second author in [46], that the numbers $S_m \in \mathcal{A}$ ($m = 1, 2, \dots$) defined by

$$(S_m)_{(p)} \;=\; \sum_{n=0}^{p-1} \frac{\mathsf{B}_n}{(-m)^n} \pmod{p}$$

in fact always belong to the subring $\mathbb{Z}$ of $\mathcal{A}$, an example being $S_9 = 14834$.

Example 7: Finite multiple zeta values. Generalizing the values of the Riemann[4] zeta function at integer arguments, one has the by now classical *multiple zeta values* (MZVs) defined by (1), where the k_i are positive integers with $k_r \geq 2$. (We should warn the reader that in many papers the same sum is denoted by $\zeta(k_r, \dots, k_1)$.) These numbers, originally introduced by Euler in the special case $r = 2$, have been extensively studied in recent years in connection with knot invariants, Feynman integrals, periods of mixed Tate motives, and other topics. We define their $\mathcal{A}$-analogues $\zeta_{\mathcal{A}}(k_1, \dots, k_r) \in \mathcal{A}$, which we will call *finite multiple zeta values* or *$\mathcal{A}$-multiple zeta values*, by

$$\zeta_{\mathcal{A}}(k_1, \dots, k_r) \;=\; \big(\zeta_p(k_1, \dots, k_r) \bmod p\big)_{p \text{ prime}} \qquad (k_1, \dots, k_r \geq 1)\,, \tag{12}$$

where $\zeta_p(k_1, \dots, k_r)$ is the truncated MZV (3). These numbers will be studied in detail in Sections 3, 4, and 6. Here are a few preliminary remarks.

1. The number $\zeta_{\mathcal{A}}(k)$ vanishes for all $k \geq 1$, even or odd, because $\sum_{n=1}^{p-1} n^{-k} \equiv 0 \bmod p$ for all $p > k+1$, so that the finite multiple zeta values give a *different* generalization of the classical single zeta values $\zeta(k)$ than the one considered in Example 5 above.

2. In fact, (12) makes sense and defines an element of $\mathcal{A}$ for any $k_1, \dots, k_r \in \mathbb{Z}$, and we will use these numbers also, but we reserve the name "finite MZV" for the case where all k_i are positive.

[4] actually, Euler

3. Here the issue of the direction of the inequalities in (3) mentioned in the first footnote almost disappears, since by sending m_i to $p - m_i$ we see immediately that $\zeta_{\mathcal{A}}(k_1, \ldots, k_r) = (-1)^{k_1+\cdots+k_r} \zeta_{\mathcal{A}}(k_r, \ldots, k_1)$.

4. Just as in the classical case, the space spanned by the $\mathcal{A}$MZVs forms a ring with respect to an appropriate shuffle product, to be discussed in detail later.

We also make some comments about terminology. The sums on the right-hand side of (3), for a fixed prime number p, have been studied by several authors ([14], [52], [38], ...), some of whose results will be quoted or discussed below. These sums are sometimes also referred to as "finite multiple zeta values." The symmetric multiple zeta values defined by (4) and studied in Parts II of this paper will also sometimes be called "finite multiple zeta values" (as in the title of the paper!) to emphasize their parallel nature to the $\mathcal{A}$MZVs, though we will then usually use the full phrase "finite real MZVs" to avoid confusion.

The key fact about the classical multiple zeta values is that they satisfy a large number of linear relations over $\mathbb{Q}$. For instance, in weight 3 and weight 4 we have the proportionality statements

$$\zeta(1,2) \;=\; \zeta(3), \qquad \zeta(1,1,2) \;=\; 4\zeta(1,3) \;=\; \frac{4}{3}\zeta(2,2) \;=\; \zeta(4)\,,$$

and more generally the dimension of the $\mathbb{Q}$-vector space $\mathfrak{Z}_k \subset \mathbb{R}$ spanned by the 2^{k-2} convergent multiple zeta values of total weight k is conjecturally equal to, and provably (by [47] and [9]) bounded above by, the number d_k defined by generating function

$$\sum_{k=0}^{\infty} d_k\, x^k \;=\; \frac{1}{1-x^2-x^3} \;=\; 1 + x^2 + x^3 + x^4 + 2x^5 + 2x^6 + 3x^7 + 4x^8 + \cdots\,. \tag{13}$$

A similar phenomenon happens also for the finite multiple zeta values. Here in weight 3 we find

$$\zeta_{\mathcal{A}}(3) = 0\,, \quad \zeta_{\mathcal{A}}(1,2) = 3Z_{\mathcal{A}}(3)\,, \quad \zeta_{\mathcal{A}}(2,1) = -3Z_{\mathcal{A}}(3)\,, \quad \zeta_{\mathcal{A}}(1,1,1) = 0$$

(so that, in particular, the $\mathcal{A}$-zeta value $Z_{\mathcal{A}}(3)$ defined above *does* occur in the ring of finite multiple zeta values, even though the more obvious analogue $\zeta_{\mathcal{A}}(3)$ of $\zeta(3)$ is 0), and similarly all finite multiple zeta values of weight 4 vanish and all finite multiple zeta values of weight 5, 6 and 7 are rational multiples of $Z_{\mathcal{A}}(5)$, $Z_{\mathcal{A}}(3)^2$ and $Z_{\mathcal{A}}(7)$ respectively. More generally, based on numerical experiments that will be discussed in §3 and theoretical considerations that will be treated in the rest of the paper, we conjecture that the dimension of the $\mathbb{Q}$-vector space $\mathfrak{Z}_{\mathcal{A},k} \subset \mathcal{A}$ spanned by the 2^{k-1} finite multiple zeta values of total weight k is given by equation (6), corresponding to the conjectural isomorphism (5).

Example 8: Zeta derivatives. Our next example, which will be used in §5, combines the ideas of Examples 3 and 5 to give the $\mathcal{A}$-analogues of the derivatives of $\zeta(s)$ at positive integers k. We start with the first derivative $\zeta'(k)$ for $k > 1$, which we define by the heuristic

$$\begin{aligned}
\zeta'(k) \;&=\; \sum_{0<n} (-\log n) n^{-k} \text{ “}\equiv\text{” } \sum_{0<n} \frac{1}{p}\bigl(1 - n^{p-1}\bigr) n^{-k} \\
&\text{“}\equiv\text{” } \frac{1}{p} \sum_{0<n} \bigl(n^{p-1-k} - n^{2p-2-k}\bigr) \\
&=\; \frac{1}{p}\bigl(\zeta(k-p+1) - \zeta(k+2-2p)\bigr) \\
&=\; \frac{1}{p}\left(-\frac{B_{p-k}}{p-k} + \frac{B_{2p-1-k}}{2p-1-k}\right),
\end{aligned}$$

leading to the definition

$$Z'_{\mathcal{A}}(k) \;:=\; \left(\frac{1}{p}\left(-\frac{B_{p-k}}{p-k}+\frac{B_{2p-1-k}}{2p-1-k}\right) \bmod p\right)_p \in \mathcal{A}\,. \tag{14}$$

Note that, just as the definitions of the $\mathcal{A}$-analogues of $\log x$ and γ used the mod p congruences of Fermat's little theorem and Wilson's theorem divided by p, the definition of $Z'_{\mathcal{A}}(k)$ uses the Kummer congruences.

Similarly, the second derivative $Z''_{\mathcal{A}}(k)$ is defined by the heuristic

$$\begin{aligned}
\zeta''(k) \;&=\; \sum_{0<n}(-\log n)^2 n^{-k} \text{ “}\equiv\text{” } \sum_{0<n}\left(\frac{1}{p}\big(1-n^{p-1}\big)\right)^2 n^{-k} \\
&\text{“}\equiv\text{” } \frac{1}{p^2}\sum_{0<n}\big(n^{p-1-k}-2n^{2p-2-k}+n^{3p-3-k}\big) \\
&=\; \frac{1}{p^2}\big(\zeta(k+1-p)-2\zeta(k+2-2p)+\zeta(k+3-3p)\big) \\
&=\; \frac{1}{p^2}\left(-\frac{B_{p-k}}{p-k}+2\frac{B_{2p-1-k}}{2p-1-k}-\frac{B_{3p-2-k}}{3p-2-k}\right)\,,
\end{aligned}$$

i.e.,

$$Z''_{\mathcal{A}}(k) \;:=\; \left(\frac{1}{p^2}\left(-\frac{B_{p-k}}{p-k}+2\frac{B_{2p-1-k}}{2p-1-k}-\frac{B_{3p-2-k}}{3p-2-k}\right) \bmod p\right)_p \in \mathcal{A}\,.$$

Of course one could do the same also for the higher derivatives, although we will not use them. We can also consider the Laurent expansion of $\zeta(s)$ at $s=1$. This is given by

$$\zeta(s) \;=\; \frac{1}{s-1}+\gamma-\gamma^{(1)}(s-1)+\cdots\,,$$

where γ is Euler's constant and $\gamma^{(1)}$ is called the Stieltjes constant. Proceeding just as above, we heuristically compute

$$\begin{aligned}
-\zeta'(1) \;&=\; \sum_{0<n}\frac{\log n}{n} \text{ “}\equiv\text{” } \frac{1}{p}\sum_{0<n}\frac{n^{p-1}-1}{n} \;=\; \frac{1}{p}\big(\zeta(2-p)-\zeta(1)\big) \\
&\equiv\; \frac{1}{p}\big(\zeta(3-2p)-\zeta(2-p)\big)\,.
\end{aligned}$$

We have $\zeta(1-m(p-1)) = -\frac{B_{m(p-1)}}{m(p-1)}$ for $m\geq 1$ by Euler, and the congruence $p\zeta(1-m(p-1)) \equiv -\frac{1}{m} \pmod p$ by von-Staudt–Clausen. Hence, we have

$$\zeta(1-m(p-1))+\frac{1}{mp} \;=\; \frac{1}{1-p}\left(\frac{B_{m(p-1)}}{m}+\frac{1-p}{mp}\right)\in\mathbb{Z}_p.$$

By Kummer (see [20]), the congruence class modulo p of this is independent of m (and is equal to the Wilson quotient modulo p), and so in particular

$$\zeta(3-2p)-\zeta(2-p) \;=\; \frac{1}{1-p}\left(\frac{1}{2}B_{2p-2}-B_{p-1}-\frac{1}{2p}+\frac{1}{2}\right)$$

is divisible by p. We therefore adopt

$$\gamma^{(1)}_{\mathcal{A}} \;=\; \left(\frac{1}{p}\Big(\frac{1}{2}B_{2p-2}-B_{p-1}-\frac{1}{2p}+\frac{1}{2}\Big) \bmod p\right)_p$$

as our definition of the $\mathcal{A}$-analogue of the Stieltjes constant.

Example 9: Numbers coming from differential equations. Define monic polynomials

$$h_k(t) \;=\; \sum_{n=0}^{k-1} c_n^{(k)}\, t^n \qquad (k \;=\; 0,\,1,\,\dots)$$

as the determinants of the upper $k\times k$ blocks of the infinite tridiagonal matrix having diagonal entries $\{n(1-n)(1+t)\}_{n\ge1}$ and near-diagonals $\{n^2t\}_{n\ge1}$ and $\{n^2\}_{n\ge1}$, or equivalently by the recursion $h_{k+1}(t)+k(k+1)(t+1)\,h_k(t)+k^4t\,h_{k-1}(t)=0$ for $k\ge1$ together with the initial values $h_0(t)=1,\ h_1(t)=0$. Then it was discovered empirically by Maxim Kontsevich some years ago that the element $c_n=\{c_n^{(p)} \bmod p\}$ of $\mathcal{A}$ always belongs to the subring $\mathbb{Q}$, with initial values given by

n	0	1	2	3	4	5	6	7
c_n	0	0	$\frac{1}{4}$	$\frac{1}{24}$	$\frac{101}{576}$	$\frac{239}{17280}$	$\frac{19153}{115200}$	$-\frac{1516283}{72576000}$

and with the numbers c_n for large n growing only exponentially in n but having numerators and denominators that grow exponentially in n^2. This was a special example of a deep theory developed by Kontsevich [28] in which the ring $\mathcal{A}$ occurred in the context of $\mathcal{D}$-modules; the specific properties of the c_n listed above were proved later by him and A. Odesskii [29] and were also studied in detail by one of the present authors.

Non-Example 10: Algebraic numbers. In our first example, we saw that all rational numbers can be considered as elements of the ring $\mathcal{A}$. We now point out that no irrational element of $\overline{\mathbb{Q}}$ can be similarly considered. For instance, if the number $\sqrt{2}$ could be represented by an element $x\in\mathcal{A}$, we would have $x_{(p)}^2\equiv 2 \pmod p$ for all sufficiently large primes p, but this congruence has no solutions for any prime congruent to $\pm3 \pmod 8$. In general, if $P(x)\in\mathbb{Z}[x]$ is an irreducible polynomial of degree >1, then a well-known and elementary argument shows that there are infinitely many primes p for which $P(x)$ has no linear factors modulo p, so no root of P can be embedded into $\mathcal{A}$. (The argument is as follows: by standard Galois theory and Chebotarev's theorem, the non-existence of infinitely many such primes would be equivalent to the statement that G is covered by the conjugates gHg^{-1} of H in G, where G and H denote the Galois groups of the normal closure of $K=\mathbb{Q}[x]/(P(x))$ over $\mathbb{Q}$ and K, respectively. But this is impossible, since H has at most $[G:H]$ conjugates, each of cardinality $|G|/[G:H]$, and they have at least one element in common.) At first sight, this statement seems to say that "the ring $\mathcal{A}$ contains no irrational algebraic elements" or that "the subring $\mathbb{Q}$ of $\mathcal{A}$ is algebraically closed," and to imply that if, for example, someone could prove an $\mathcal{A}$-analogue of Apéry's famous result $\zeta(3)\notin\mathbb{Q}$, then it would follow that such an element is transcendental. This conclusion, however, is not true: $\mathbb{Q}$ *is* algebraically closed in $\mathcal{A}$ in the sense that no irrational element of its usual closure $\overline{\mathbb{Q}}$ can be embedded into $\mathcal{A}$, but *not* in the sense that elements of $\mathcal{A}\setminus\mathbb{Q}$ cannot be the roots of any polynomials with rational coefficients. The reason is that $\mathcal{A}$ has many zero-divisors, so that these two statements, which are equivalent within (say) $\mathbb{C}$, are not at all equivalent here. For example, if we define $\alpha\in\mathcal{A}$ by taking its p-component to be one of the two square-roots of $2 \pmod p$ whenever p is congruent to $\pm1 \pmod 8$ and to be 0 whenever p is congruent to $\pm3 \pmod 8$, then α is algebraic over $\mathbb{Q}$ in the sense that it satisfies the polynomial equation $\alpha(\alpha^2-2)=0$ in $\mathcal{A}$, but it is not the root of any irreducible polynomial in $\mathbb{Q}[x]$. We mention this just as a warning that more care must be taken when working with numbers in $\mathcal{A}$ than when working over the complex numbers.

However, these problems can in fact be overcome and a correct analogue of algebraic numbers in the ring $\mathcal{A}$ was defined by J. Rosen [41]. See also Rosen-Takeyama-Tasaka-Yamamoto [42].

Computing in the ring $\mathcal{A}$. To find experimentally results such as equation (7) or (9), we need an efficient algorithm to find linear relations over $\mathbb{Q}$ among given elements of the ring $\mathcal{A}$. We end this section with a brief discussion of how to do this. Recall that the corresponding problem over $\mathbb{R}$, i.e., the problem of finding numerically relations $\sum_{i=1}^{N} n_i x_i = 0$ with integers n_i of reasonable size if one is given a collection of real numbers x_i to sufficiently high precision, is solved by the famous LLL (Lenstra-Lenstra-Lovasz) lattice reduction algorithm, which is efficiently pre-programmed in many high-level mathematical software packages such as PARI-GP (where one simply types "`lindep(x)`," x being the vector with components x_i, and gets the vector of n_i as output). It turns out that one can solve the problem over $\mathcal{A}$ just as easily as an application of the real version. The idea is very simple. We first compute the p-components $(x_i)_{(p)}$ of x_i for all primes p in some interval $[A, B]$ which is not too long for computations but is sufficiently big that the product P of all primes in the interval is very large. (Typical values might be $A = 30$, $B = 500$, for which $P \approx 2 \times 10^{196}$.) We then use the Chinese remainder theorem (which is also efficiently pre-programmed in PARI and many other high-level mathematical software programs) to lift these collections of residue classes to residue classes $X_i \in \mathbb{Z}/P\mathbb{Z}$, where we can represent each X_i by an integer in the interval $[-P/2, P/2]$. Usually, all of these integers will then be of the same order of magnitude as P (unless, of course, one of the numbers on our list $\{x_i\}$ was 1, in which case the corresponding X_i will also be 1; this case must be treated separately). Now assume that there is a relation $\sum n_i x_i = 0$ in $\mathcal{A}$ with integral coefficients n_i that are not too large. We can assume that the corresponding congruence $\sum n_i (x_i)_{(p)} \equiv 0 \pmod{p}$ holds for all $p \in [A, B]$, either by assuming (after varying A if necessary) that the lower limit A of our chosen interval is sufficiently large to avoid exceptional primes where the congruence fails or else by the simple expedient of multiplying all n_i by any prime p where it fails. We then have $\sum n_i X_i = n_0 P$ with an integer n_0 of the same order of magnitude as the coefficients n_i of the (as yet unknown) relation. Now we simply divide by P and write the relation as $-n_0 + \sum_i n_i (X_i/P) = 0$, so by applying the *real* LLL-algorithm to the vector of numbers $(-1, X_1/P, \ldots, X_N/P)$ one finds the desired integers n_i. (In the important already-mentioned special case $X_1 = 1$, the number X_1/P, being very close to 0, will be missed by the real LLL algorithm, but once one has the other n_i one finds n_1 from the relation.) This works extremely well in practice and the calculations with, for example, $\mathcal{A}$-multiple zeta values are actually much easier and quicker to carry out than corresponding calculations with the more familiar real ones.

2. Sun's harmonic moment sums

As a gentle introduction to the general case, in this section we discuss the computation of the numbers $V(i,j)$ defined for $i \in \mathbb{Z}$ and $j \in \mathbb{Z}_{\geq 0}$ by the harmonic moment sums (8) and the proof of numerical relations like equation (9). Using the numerical method just described for calculating in the ring $\mathcal{A}$, we find (numerically, but to very high precision) the values tabulated in Table 1 in the range $|i| \leq 6$, $j \leq 6$, with the trivial values $V(i,0) = -\delta_{i,0}$ omitted. Studying these and many further values gave rise to the following observations:

(i) For $i < 0$, the value of $V(i,j)$ is a homogeneous element of weight $|i| + j$ in $\mathfrak{Z}_{\mathcal{A}}$. For instance, the number $Z_k = V(1-k,1)$ is always equal to $k\,Z_{\mathcal{A}}(k)$ with $Z_{\mathcal{A}}(k)$ as in (11), and the number $Y_k = V(2-k,2)$ (k even) is always equal to $2\zeta_{\mathcal{A}}(1,1,k-2)$.

(ii) The subspace $\mathfrak{V}_k \subset \mathfrak{Z}_{\mathcal{A},k}$ spanned by the $k-1$ elements $V(j-k,j)$ $(1 \leq j \leq k-1)$ has dimension smaller than $k/2$ for all $k \geq 1$.

(iii) One has $V(1,j) = -\frac{1}{2}V(0,j)$ for all $j \geq 1$.

(iv) The number $V(i,1)$ for $i \geq 0$ equals B_i, the ith Bernoulli number.

(v) The numbers $V(i,2)$ and $V(i,3)$ are also rational for all $i \geq 0$, the numbers $V(i,4)$ and $V(i,5)$ are rational linear combinations of 1 and $Z_{\mathcal{A}}(3)$, and the numbers $V(i,6)$ are rational linear combinations of 1, $Z_{\mathcal{A}}(3)$, and $Z_{\mathcal{A}}(5)$. More generally, the elements $V(i,j)$ for fixed j and all $i \geq 0$ belong to the finite-dimensional space $\mathbb{Q} + \mathfrak{V}_1 + \cdots + \mathfrak{V}_{j-1}$.

(vi) The degree $j-1$ component of $V(i,j)$ for $i \geq 0$ is proportional to B_i for each j, e.g., the weight 3 part of $V(i,4)$ is always $2B_iZ_3$, the weight 5 part of $V(i,6)$ is always $29\,B_iZ_5$, and the weight 8 part of $V(i,9)$ is always $B_i\,(987\,Z_3Z_5 - \frac{933}{2}\,Y_8)$.

$i \setminus j$	1	2	3	4	5	6
-6	Z_7	Y_8	$\frac{359}{108}Z_9 + \frac{1}{9}Z_3^3$	$\frac{247}{16}Y_{10} + \frac{49}{8}Z_3Z_7 + \frac{27}{16}Z_5^2$		
-5	0	Z_7	$\frac{3}{2}Y_8$	$\frac{305}{54}Z_9 + \frac{2}{9}Z_3^3$	$\frac{1155}{32}Y_{10} + \frac{245}{16}Z_3Z_7 + \frac{135}{32}Z_5^2$	
-4	Z_5	$-\frac{1}{3}Z_3^2$	$\frac{25}{8}Z_7$	$\frac{47}{2}Y_8 + 11Z_3Z_5$	$\frac{8281}{324}Z_9 - \frac{10}{27}Z_3^3$	$\frac{2061}{8}Y_{10} + 102Z_3Z_7 + \frac{505}{8}Z_5^2$
-3	0	Z_5	$-\frac{1}{2}Z_3^2$	$\frac{21}{4}Z_7$	$\frac{225}{4}Y_8 + \frac{55}{2}Z_3Z_5$	$\frac{1135}{18}Z_9 - \frac{5}{3}Z_3^3$
-2	Z_3	0	$\frac{7}{2}Z_5$	$\frac{2}{3}Z_3^2$	$\frac{279}{8}Z_7$	$\frac{223}{4}Y_8 + \frac{113}{2}Z_3Z_5$
-1	0	Z_3	0	$6Z_5$	$\frac{5}{2}Z_3^2$	$92Z_7$
0	1	-2	6	$[-24,\ 2]$	$[120,\ -10]$	$[-720,\ 60,\ 29]$
1	$-\frac{1}{2}$	1	-3	$[12,\ -1]$	$[-60,\ 5]$	$[360,\ -30,\ -\frac{29}{2}]$
2	$\frac{1}{6}$	$-\frac{4}{9}$	$\frac{23}{18}$	$[-\frac{136}{27},\ \frac{1}{3}]$	$[\frac{2030}{81},\ -\frac{20}{9}]$	$[-\frac{12160}{81},\ \frac{112}{9},\ \frac{29}{6}]$
3	0	$\frac{1}{6}$	$-\frac{5}{12}$	$[\frac{14}{9},\ 0]$	$[-\frac{205}{27},\ \frac{5}{6}]$	$[\frac{1220}{27},\ -\frac{11}{3},\ 0]$
4	$-\frac{1}{30}$	$-\frac{7}{225}$	$\frac{217}{2250}$	$[-\frac{4177}{16875},\ -\frac{1}{15}]$	$[\frac{53906}{50625},\ -\frac{7}{45}]$	$[-\frac{1530311}{253125},\ \frac{142}{225},\ -\frac{29}{30}]$
5	0	$-\frac{1}{30}$	$-\frac{7}{150}$	$[\frac{59}{2250},\ 0]$	$[-\frac{26}{3375},\ -\frac{1}{6}]$	$[-\frac{6563}{33750},\ -\frac{7}{15},\ 0]$
6	$\frac{1}{42}$	$\frac{76}{2205}$	$\frac{11071}{308700}$	$[-\frac{1768957}{16206750},\ \frac{1}{21}]$	$[\frac{132639347}{340341750},\ \frac{76}{441}]$	$[-\frac{26513619449}{11911961250},\ \frac{8108}{15435},\ \frac{29}{42}]$
	1	1	1	$[1,\ Z_3]$	$[1,\ Z_3]$	$[1,\ Z_3,\ Z_5]$

Table 1. In this table Z_k and Y_k denote $V(1-k,1)$ and $V(2-k,2)$, respectively.

We now prove each of these properties. Statement (i) is easy, because for $h > 0$ we have

$$V(-h,j)_{(p)} \;\equiv\; \sum_{0<n_1,\dots,n_j \leq n < p} \frac{1}{n_1\,\cdots\,n_j\,n^h} \qquad (\mathrm{mod}\ p)\,.$$

By considering all possible combinations of equalities and inequalities among the numbers $n_1,\dots,n_j,n$, we see that this is a weight $h+j$ element of the ring $\mathfrak{Z}_{\mathcal{A}}$.

For (ii), we note first that the subspace $\mathfrak{V}_k \subset \mathfrak{Z}_{\mathcal{A},k}$ defined there has dimension $\le k-1$ by its very definition. The better dimension bound in (ii) will follow from the three identities

$$\begin{aligned} \sum_{j=r}^{2r}(-1)^j\binom{r}{j-r}V(j-k,j) &= 0 \quad \text{if } k \text{ is odd},\\ \sum_{j=r}^{2r+1}(-1)^j\left(\binom{r}{j-r-1}+\binom{r+1}{j-r}\right)V(j-k,j) &= 0 \quad \text{if } k \text{ is even} \end{aligned} \tag{15}$$

and

$$\sum_{j=0}^{m}(-2)^j\binom{m}{j}V(j-k,j) \;=\; 0 \quad \text{if } m\not\equiv k \pmod 2, \tag{16}$$

all of which we found experimentally and will prove as corollaries to Proposition 2 below. Equation (15) gives the desired upper bound because reading it from the bottom up or from the top down gives the two spanning sets

$$\bigl\{V(j-k,j)\mid k/2<j<k\bigr\} \quad \text{or} \quad \bigl\{V(j-k,j)\mid 0<j<k,\ j\equiv k \pmod 2\bigr\} \tag{17}$$

by using it recursively to write any $V(j-k,j)$ with $0<j<k$ as a linear combination of $V(j'-k,j')$ with $j'>j$ if $j=r<k/2$ and as a linear combination of $V(j'-k,j')$ with $j'<j$ if $j=2r$ or $2r-1$ is different from k (mod 2). Equation (16) will also give a third proof of (ii), with a different spanning set of the same cardinality as those in (17) but with nicer properties.

We observe that for small values of k the upper bound $\left[\frac{k-1}{2}\right]$ is too large (for instance, there are no $\mathcal{A}$MZVs of weight 4 in Table 1 and only one each of weights 5, 6 or 7), simply because $\mathfrak{V}_k$ is contained in $\mathfrak{Z}_{\mathcal{A},k}$, whose dimension is smaller. Statement (i) and (ii) together imply that

$$\dim\mathfrak{V}_k \;\le\; \min\Bigl\{\dim\mathfrak{Z}_{\mathcal{A},k},\,\Bigl[\frac{k-1}{2}\Bigr]\Bigr\} \;=\; \begin{cases}\dim\mathfrak{Z}_{\mathcal{A},k} & \text{if } k\le 11,\\ \left[\frac{k-1}{2}\right] & \text{if } k\ge 12.\end{cases} \tag{18}$$

We conjecture, and have checked numerically to high precision up to weight 30, that this inequality is in fact always an equality. In the same context, we should point out that the subspace $\mathbb{Q}\oplus\sum_{k>0}\mathfrak{V}_k$ of $\mathfrak{Z}_{\mathcal{A}}$ looks like a subalgebra in the range contained in Table 1, but this is simply because it coincides with all of $\mathfrak{Z}_{\mathcal{A}}$ in weights up to 11. In fact, it is not a subring (or at least, not numerically to very high $\mathcal{A}$-precision), since for instance the product $V(-4,2)V(-6,1)$ of weight 13 is not (at least numerically) in the $\mathbb{Q}$-span $\mathfrak{V}_{13}$ of $V(-12,1),\dots,V(-1,12)$.

The proof of (iii) is again easy, since from $H_n\equiv H_{p-1}-(-H_{p-1-n})\equiv H_{p-1-n} \pmod p$ we get

$$2\,V(1,j)_{(p)} \;\equiv\; \sum_{0<n<p}(n\,+\,n)\,H_n^j \;\equiv\; \sum_{0<n<p}(n\,+\,(p-1-n))\,H_n^j \;\equiv\; -V(0,j)_{(p)}\,.$$

For property (iv) we use Fermat's little theorem, the Seki-Bernoulli formula[5] for the sum of fixed powers of the first n integers, and the obvious formula $\binom{p-1}{\ell}\equiv(-1)^\ell \pmod p$ for $0\le\ell<p$, to

[5] Both the "Bernoulli numbers" and the formula for the sum of the first n powers of any fixed degree were discovered independently at about the same time by Takakazu Seki (16??–1708) and Jakob Bernoulli (1654–1705).

see that the harmonic sum H_n for $n < p$ is given modulo p by

$$\begin{aligned} H_n &= 1 + \frac{1}{2} + \cdots + \frac{1}{n} \equiv 1^{p-2} + 2^{p-2} + \cdots + n^{p-2} \\ &= \frac{1}{p-1}\sum_{\ell=0}^{p-2}(-1)^\ell \binom{p-1}{\ell} B_\ell\, n^{p-1-\ell} \equiv -\sum_{\ell=0}^{p-2}\frac{B_\ell}{n^\ell}, \end{aligned} \tag{19}$$

where all congruences are modulo p. It follows immediately that

$$V(i,1)_{(p)} \equiv \sum_{n=1}^{p-1} n^i H_n \equiv -\sum_{n=1}^{p-1}\sum_{\ell=0}^{p-2} B_\ell\, n^{i-\ell} \equiv \sum_{\ell=0}^{p-2} B_\ell\, \delta_{\ell,i} = B_i$$

for $0 \le i \le p-2$, and hence that $V(i,1) = B_i$ in $\mathcal{A}$, as claimed.

For properties (v) and (vi), we further have found a considerable generalization. We now state this together with all the properties already proven in a single theorem.

Theorem 1. (1) *All Sun sums $V(i,j)$ $(i \in \mathbb{Z}, j \ge 0)$ belong to $\mathfrak{Z}_\mathcal{A}$. Furthermore, the weight k part $V(i,j)^{(k)}$ of every $V(i,j)$ belongs to a subspace $\mathfrak{V}_k$ of $\mathfrak{Z}_{\mathcal{A},k}$ of dimension $< k/2$ if $k > 0$.*

(2) *For $i < 0$, the elements $V(i,j)$ are homogeneous of weight $k = j + |i|$, and the $k-1$ elements $V(j-k,j)$ $(0 < j < k)$ span the space $\mathfrak{V}_k$.*

(3) *For $i \ge 0$, the weight k part $V(i,j)^{(k)}$ of $V(i,j)$ vanishes for $k \ge j$, while for $k = j-r < j$, it is a rational linear combination of $X_\nu^{(k)}$ with $0 \le \nu < r/2$, where $X_\nu^{(k)}$ $(0 \le \nu < k/2)$ are elements independent of r and j, that span the space $\mathfrak{V}_k$. More precisely, we have*

$$\frac{1}{j!}V(i,j)^{(k)} = \sum_{0\le\nu<r/2} B_i^{(r,\nu)} X_\nu^{(k)} \quad (r := j-k) \tag{20}$$

where the $B_i^{(r,\nu)}$ are rational numbers independent of k that vanish for $i < 2\nu$.

Remark. The last formula (20) is a very strong statement, in two different ways. On the one hand, it says that the infinitely many elements $V(i,k+1)^{(k)}$ $(i = 0,1,2,...)$ for fixed k are rational multiples of a single vector $X_0^{(k)} \in \mathfrak{V}_k$, the infinitely many elements $V(i,k+2)^{(k)}$ are rational multiples of the same vector, the infinitely many elements $V(i,k+3)^{(k)}$ and $V(i,k+4)^{(k)}$ are rational linear combinations of that vector and a second vector $X_1^{(k)} \in \mathfrak{V}_k$, etc. The first of these assertions is half of the first observation in (vi) at the beginning of the section, with $X_0^{(5)} = 29Z_5$ and $X_0^{(8)} = 987\,Z_3Z_5 - \frac{933}{2}Y_8$. On the other hand, the second half of (vi) said that the rational number $V(i,k+1)^{(k)}/X_0^{(k)}$ is equal to the i-th Bernoulli number B_i, independent of k. The generalization of this is that the coefficient of each basis element $X_\nu^{(k)}$ in $V(i,k+r)^{(k)}$ is a rational number $B_i^{(r,\nu)}$ depending on r,ν and i but not on k.

Proof. We have already proved (1) and (2) (under Proposition 2). The rest of this section is devoted to the proof of (3), which will mostly depend on the following identity, which determines the numbers $V(i,j)$ recursively and which will be proved below as a consequence of Proposition 2.

Proposition 1. *For $i \ge 0$ and $j \ge 1$, we have*

$$V(i,j) = \frac{1}{i+1}\left(\sum_{h=1}^{j-1}(-1)^h\binom{j}{h} V(i+1-h,j-h) - (-1)^j\delta_{i+1,j} - \sum_{i'=0}^{i-1}\binom{i+1}{i'} V(i',j)\right). \tag{21}$$

In terms of the generating series

$$\mathcal{V}_j(x) \;:=\; \sum_{i=0}^{\infty} V(i,j)\,\frac{x^i}{i!} \quad\in\quad \mathcal{A}[[x]] \qquad (\forall j \ge 0),$$

this is equivalent to the identity

$$(e^x - 1)\,\mathcal{V}_j(x) \;=\; \sum_{h=1}^{j}(-1)^h\binom{j}{h}\sum_{i=0}^{\infty} V(i-h,j-h)\,\frac{x^i}{i!}\,. \tag{22}$$

Differentiating this $j-1$ times with respect to x and replacing h by $j-h$, we obtain a differential recursion for the power series $\mathcal{V}_j(x)$:

$$\frac{d^{j-1}}{dx^{j-1}}\big[(e^x - 1)\,\mathcal{V}_j(x)\big] \;=\; \sum_{h=1}^{j-1}(-1)^{j-h}\binom{j}{h}\,\frac{d^{h-1}}{dx^{h-1}}\mathcal{V}_h(x) \;+\; (-1)^{j-1}x\,. \tag{23}$$

Before proceeding, let us now compute $\mathcal{V}_j(x)$ for small j using these equations. For $j=1$, equation (22) immediately gives

$$\mathcal{V}_1(x) \;=\; \frac{x}{e^x-1}\,, \tag{24}$$

giving another proof of (iv). For $j=2$, equations (23) and (24) give

$$\frac{d}{dx}\big[(e^x-1)\,\mathcal{V}_2(x)\big] \;=\; -\,2\,\mathcal{V}_1(x) \,-\, x \qquad \Big(=\,-\,x\,\frac{e^x+1}{e^x-1}\Big)\,,$$

and integrating this we find

$$(e^x-1)\,\mathcal{V}_2(x) \;=\; -2\,\mathrm{Li}_2\big(1-e^{-x}\big) \,-\, \frac{x^2}{2}\,, \tag{25}$$

where $\mathrm{Li}_2(z) = \sum_{m=1}^{\infty} z^m/m^2$ is the classical dilogarithm series. In terms of the "modified poly-Bernoulli numbers" introduced in [2], which are the rational numbers $C_n^{(k)}$ defined by

$$\frac{\mathrm{Li}_k(1-e^{-t})}{e^t-1} \;=\; \sum_{n=0}^{\infty} C_n^{(k)}\frac{t^n}{n!}, \tag{26}$$

(where $\mathrm{Li}_k(z) = \sum_{m=1}^{\infty} z^m/m^k$ is the kth polylogarithm), we can rewrite (25) as the formula

$$V(i,2) \;=\; -\frac{i}{2}\,B_{i-1} \,-\, 2\,C_i^{(2)} \tag{27}$$

for the numbers $V(i,2)$. Note that, $C_i^{(2)} = -\frac{i+2}{4}B_{i-1}$ if i is odd, as can be seen by writing the generating series as

$$\frac{\mathrm{Li}_k(1-e^{-t})}{e^t-1} \;=\; \frac{1}{e^t-1}\int_0^t \frac{x}{e^x-1}\,dx$$

and expanding the right-hand side, so $V(i,2) = B_{i-1}$ if i is odd, as we see for $i \le 6$ in Table 1. By (15) with $r=2$ and k even, we have

$$V(i,3) \;=\; \frac{3}{2}V(i-1,2) + \frac{1}{4}\delta_{i,3} \;=\; -3C_{i-1}^{(2)} + \delta_{i,3} \quad (i>0,\ \text{odd}).$$

This determines $\mathcal{V}_3^{(-)}(x)$, where $\mathcal{V}_j^{(-)}(x)$ and $\mathcal{V}_j^{(+)}(x)$ denote the odd and even parts of the power series $\mathcal{V}_j(x)$. But Proposition 2 below (evenness of $e^{x/2}\mathcal{V}_j(x)$) implies that

$$\mathcal{V}_j^{(+)}(x) \;=\; -\frac{e^x+1}{e^x-1}\,\mathcal{V}_j^{(-)}(x). \tag{28}$$

This therefore determines $V(i,3)$ completely for all i, and shows that it is always a rational number. Similarly, by (15) with $r=2$ and k odd, we have

$$\widehat{\mathcal{V}_4^{(-)}}(z) \;=\; 2\widehat{\mathcal{V}_3^{(+)}}(z)\,z - \widehat{\mathcal{V}_2^{(-)}}(z)\,z^2 \;-\; Z_3\,z\,,$$

where for any power series $f(x)=\sum_{n=0}^{\infty} a_n \frac{x^n}{n!}$, we denote by $\widehat{f}(z)$ its Laplace transform defined by $\widehat{f}(z)=\sum_{n=0}^{\infty} a_n z^n$. This and (28) determines $\mathcal{V}_4(x)$ completely, and shows that every $V(i,4)$ is a $\mathbb{Q}$-linear combination of 1 and $Z_{\mathcal{A}}(3)$, as asserted in (v). The general statement of (v) (or (3) of Theorem 1) that any $V(i,j)$ for $i\geq 0$ is in the space spanned by $\mathcal{A}$MZVs of weight strictly less than j is seen either from the formula (21) using the induction on j (and on i), or directly (as in the proof of (i)) from the expression

$$V(i,j)_{(p)} \;\equiv\; \sum_{0<n_1,\dots,n_j\leq n<p} \frac{n^i}{n_1\,\cdots\,n_j} \qquad \pmod{p}\,,$$

and the Seki-Bernoulli formula.

To prove equation (21) and the formula (20) in the theorem, we introduce two other generating series

$$\begin{aligned} \mathcal{U}_k(x) \;&:=\; \sum_{j=0}^{\infty} V(j-k,j)\frac{x^j}{j!} \quad\in\; \mathcal{A}[[x]] \qquad (\forall k\in\mathbb{Z}),\\ \mathcal{W}_j(z) \;&:=\; \sum_{h=-\infty}^{\infty} V(j-h,j)z^{-h} \quad\in\; \mathcal{A}[[z^{-1},z]] \qquad (\forall j\geq 0), \end{aligned} \tag{29}$$

Note that $\mathcal{U}_0(x) = \mathcal{W}_0(z) = -1$ (constant power series). The following two even/oddness properties of $\mathcal{U}_k(x)$ and $\mathcal{V}_j(x)$, although the proofs are very simple, are the core of our whole investigation of Sun sums.

Proposition 2. *The power series $e^{-x/2}\mathcal{U}_k(x)$ is even or odd if k is even or odd respectively. The power series $e^{x/2}\mathcal{V}_j(x)$ is even for all $j\geq 1$.*

Proof. By the congruence $H_n \equiv H_{p-1-n} \pmod{p}$ used above, we have

$$V(j-k,j)_{(p)} \;\equiv\; \sum_{0<n<p} n^{j-k}H_{p-1-n}^j \equiv \sum_{0<n<p} (-n)^{j-k}H_{n-1}^j \pmod{p},$$

from which it follows that

$$\mathcal{U}_k(x)_{(p)} \;=\; \sum_{0<n<p} (-n)^{-k}e^{-nH_{n-1}x} \;=\; (-1)^k\sum_{0<n<p} n^{-k}e^{-n(H_n-1/n)x} \;=\; (-1)^k\mathcal{U}_k(-x)_{(p)}e^x$$

and hence $e^{-x/2}\mathcal{U}_k(x) \;=\; (-1)^k e^{x/2}\mathcal{U}_k(-x)$ as claimed. Similarly, we have

$$V(i,j)_{(p)} \;\equiv\; \sum_{0<n<p} n^iH_{p-1-n}^j \equiv \sum_{0<n<p} (-n)^iH_{n-1}^j \pmod{p},$$

and hence

$$\mathcal{V}_j(x)_{(p)} \;=\; \sum_{0<n<p} e^{-nx}H_{n-1}^j \;\equiv\; \sum_{0<n<p} e^{-nx-x}H_n^j = e^{-x}\mathcal{V}_j(-x)_{(p)},$$

from which the evenness of $e^{x/2}\mathcal{V}_j(x)$ follows. □

From the proposition, we can write

$$e^{-x/2}\mathcal{U}_k(x) \;=\; \sum_{m=0}^{\infty} U(k,m)\,x^m$$

for some coefficients $U(k,m) \in \mathcal{A}$ with $U(k,m)=0$ if $m \not\equiv k \pmod 2$. Equivalently,

$$V(j-k,j) \;=\; j!\sum_{m=0}^{j} \frac{2^{m-j}}{(j-m)!}\,U(k,m). \tag{30}$$

Conversely, the $U(k,m)$ can be written in terms of $V(j-k,j)$ as

$$U(k,m) \;=\; \frac{1}{m!}\sum_{j=0}^{m}(-2)^{m-j}\binom{m}{j}V(j-k,j), \tag{31}$$

from which the recursion (16) follows. Also, since we know the elements $V(j-k,j)$ $(0<j<k)$ are homogeneous of weight $k>0$, the same is true for $U(k,m)$ $(0<m<k, m\equiv k \pmod 2)$ and we have the following corollary.

Corollary 1. *The $k-1$ numbers $V(j-k,j) \in \mathfrak{Z}_{\mathcal{A},k}$ $(j=1,\ldots,k-1)$ can be written as rational linear combinations of $\left[\frac{k-1}{2}\right]$ numbers*

$$\bigl\{U(k,m) \mid 0<m<k,\ m\equiv k \pmod 2\bigr\}. \tag{32}$$

In a different direction, by comparing the coefficients of $x^j/j!$ on both sides of the identity $(-1)^h\mathcal{U}_h(-x) = e^{-x}\mathcal{U}_h(x)$, we get the following corollary.

Corollary 2. *For all $i \in \mathbb{Z}$ and $j \geq 0$ we have*

$$(-1)^i V(i,j) \;=\; \sum_{h=0}^{j}(-1)^h\binom{j}{h}V(i-h,j-h)\,. \tag{33}$$

The identity (22) (and hence Proposition 1) follows immediately from this because we have

$$\mathcal{V}_j(-x) \;=\; \sum_{h=0}^{j}(-1)^h\binom{j}{h}\sum_{i=0}^{\infty}V(i-h,j-h)\frac{x^i}{i!},$$

and the left-hand side of this is equal to $e^x\mathcal{V}_j(x)$ by Proposition 2, and thus we have (22).

We now prove the equations (15) stated near the beginning of this section. These identities are equivalent (by comparing the coefficients of z^{-k} on both sides) to the power series identities

$$\begin{aligned}
&\sum_{\nu=0}^{r}(-1)^\nu\binom{r}{\nu}\mathcal{W}^{(-)}_{j-\nu}(z) \;=\; 0 \qquad \text{if} \quad j=2r\geq 0,\\
&\sum_{\nu=0}^{r+1}(-1)^\nu\left(\binom{r}{\nu}+\binom{r+1}{\nu}\right)\mathcal{W}^{(+)}_{j-\nu}(z) = 0 \qquad \text{if} \quad j=2r+1\geq 1.
\end{aligned} \tag{34}$$

Here are some examples.

Example 1.

$$\begin{aligned}\mathcal{W}_0^{(-)}(z) &= 0,\\ 2\mathcal{W}_1^{(+)}(z)-\mathcal{W}_0^{(+)}(z) &= 0,\\ \mathcal{W}_2^{(-)}(z)-\mathcal{W}_1^{(-)}(z) &= 0,\\ 2\mathcal{W}_3^{(+)}(z)-3\mathcal{W}_2^{(+)}(z)+\mathcal{W}_1^{(+)}(z) &= 0,\\ \mathcal{W}_4^{(-)}(z)-2\mathcal{W}_3^{(-)}(z)+\mathcal{W}_2^{(-)}(z) &= 0,\\ 2\mathcal{W}_5^{(+)}(z)-5\mathcal{W}_4^{(+)}(z)+4\mathcal{W}_3^{(+)}(z)-\mathcal{W}_2^{(+)}(z) &= 0,\\ \mathcal{W}_6^{(-)}(z)-3\mathcal{W}_5^{(-)}(z)+3\mathcal{W}_4^{(-)}(z)-\mathcal{W}_3^{(-)}(z) &= 0.\end{aligned} \tag{35}$$

To prove (34), we use the formula (30). For $j=2r$, we have

$$\begin{aligned}\sum_{\nu=0}^{r}(-1)^\nu\binom{r}{\nu}\mathcal{W}_{j-\nu}^{(-)}(z) &= \sum_{\nu=0}^{r}(-1)^\nu\binom{r}{\nu}\sum_{\substack{h\in\mathbb{Z}\\ h:\text{odd}}}V(j-\nu-h,j-\nu)z^{-h}\\ &= \sum_{\substack{h\in\mathbb{Z}\\ h:\text{odd}}}z^{-h}\sum_{\nu=0}^{r}(-1)^\nu\binom{r}{\nu}(j-\nu)!\sum_{m=0}^{j-\nu}\frac{2^{m+\nu-j}}{(j-\nu-m)!}U(h,m)\\ &= \sum_{\substack{h\in\mathbb{Z}\\ h:\text{odd}}}z^{-h}\sum_{m=0}^{j}2^{m-j}m!\,U(h,m)\sum_{\nu=0}^{r}(-2)^\nu\binom{r}{\nu}\binom{j-\nu}{m}.\end{aligned}$$

The innermost sum is equal to

$$\frac{1}{m!}\frac{d^m}{dx^m}(x-2)^r x^r\bigg|_{x=1} = \frac{1}{m!}\frac{d^m}{dy^m}(y^2-1)^r\bigg|_{y=0}$$

(here we have set $x=y+1$) and this is 0 because $(y^2-1)^r$ is an even polynomial and m is odd. Likewise, when $j=2r+1$, the left-hand side of (34) becomes

$$\sum_{\substack{h\in\mathbb{Z}\\ h:\text{even}}}z^{-h}\sum_{m=0}^{j}2^{m-j}m!\,U(h,m)\sum_{\nu=0}^{r+1}(-2)^\nu\left(\binom{r}{\nu}+\binom{r+1}{\nu}\right)\binom{j-\nu}{m}$$

and the innermost sum of this is equal to

$$\frac{1}{m!}\frac{d^m}{dx^m}\left((x-2)^r x^{r+1}+(x-2)^{r+1}x^r\right)\bigg|_{x=1} = \frac{2}{m!}\frac{d^m}{dy^m}y(y^2-1)^r\bigg|_{y=0},$$

which is 0 because this time $y(y^2-1)^r$ is odd and m is even. This completes the proof of (34) and hence (15).

Now we prove (20), which, in terms of generating series, is equivalent to the formula

$$\frac{\mathcal{V}_j^{(k)}(x)}{j!} = \sum_{0\le\nu<\min(r,k)/2}B_{r,\nu}(x)\,X_\nu^{(k)}\quad(j=k+r>k\ge 0), \tag{36}$$

where $B_{r,\nu}(x) \in \mathbb{Q}[[x]]$ and $X_\nu^{(k)} \in \mathfrak{V}_k$ are defined as follows. The power series $B_{r,\nu}(x)$ are defined recursively for each fixed value of $\nu \ge 0$ by

$$(e^x-1)B_{r,\nu}(x) \;=\; \sum_{n=1}^{r-1-2\nu} \frac{(-1)^n}{n!} I^n(B_{r-n,\nu}(x)) \;+\; (4\nu+1)(2\nu)!\frac{\binom{r-1}{2\nu}}{(r+2\nu)!}\frac{(-x)^r}{r!}. \tag{37}$$

Here, $I^n(f(x))$ for a power series $f(x)=\sum_{m=0}^\infty a_m x^m/m!$ is the n-times iteration of the formal integration: $I^n(f(x))=\sum_{m=0}^\infty a_m x^{m+n}/(m+n)!$. In particular, the "initial value" $B_{2\nu+1,\nu}(x)$ is given by

$$B_{2\nu+1,\nu}(x) \;=\; -\frac{1}{(2\nu+1)(4\nu)!}\frac{x^{2\nu+1}}{e^x-1}, \tag{38}$$

and each $B_{r,\nu}(x)$ begins

$$B_{r,\nu}(x) \;=\; \frac{(-1)^r x^{2\nu}}{(4\nu)!(2\nu+1)^{r-2\nu}} \;+\; \cdots \in \mathbb{Q}[[x]] \quad (r>0,\ 0\le \nu < r/2).$$

It is true, but not at all obvious, that each $B_{r,\nu}(x)$ is $e^{-x/2}$ times an *even* power series, the first few cases being listed in the following table: This evenness is compatible with Proposition 2

(r,ν)	$(-1)^r e^{x/2} B_{r,\nu}(x)$
$(1,0)$	$1-\frac{1}{24}x^2+\frac{7}{5760}x^4-\frac{31}{967680}x^6+\frac{127}{154828800}x^8-\cdots$
$(2,0)$	$1-\frac{1}{72}x^2-\frac{19}{86400}x^4+\frac{1831}{101606400}x^6-\frac{419}{602112000}x^8+\cdots$
$(3,0)$	$1-\frac{1}{54}x^2+\frac{493}{1296000}x^4-\frac{67877}{5334336000}x^6+\frac{2382881}{5120962560000}x^8-\cdots$
$(3,1)$	$\frac{1}{72}x^2-\frac{1}{1728}x^4+\frac{7}{414720}x^6-\frac{31}{69672960}x^8+\cdots$
$(4,0)$	$1-\frac{13}{648}x^2+\frac{6479}{19440000}x^4-\frac{5378159}{1120210560000}x^6+\cdots$
$(4,1)$	$\frac{1}{216}x^2+\frac{1}{25920}x^4-\frac{59}{8709120}x^6+\frac{937}{3135283200}x^8-\cdots$
$(5,0)$	$1-\frac{5}{243}x^2+\frac{98437}{291600000}x^4-\frac{341336357}{58811054400000}x^6+\cdots$
$(5,1)$	$\frac{1}{648}x^2-\frac{83}{5443200}x^4+\frac{583}{457228800}x^6-\frac{174863}{1975228416000}x^8+\cdots$
$(5,2)$	$\frac{1}{201600}x^4-\frac{1}{4838400}x^6+\frac{1}{165888000}x^8-\cdots$

and the formula (36) above, and would follow from them if we knew that $X_\nu^{(k)}$ are linearly independent (apart from the relation (44)), but can also be proved directly. The sketch of proof is as follows. For an arbitrary given sequence $\{a_r\}_{r\ge1}$, consider the sequence of power series $C_r(x)$ $(r\ge1)$ determined uniquely by the recursion

$$(e^x-1)C_r(x) \;=\; \sum_{n=1}^{r-1}\frac{(-1)^n}{n!}I^n(C_{r-n}(x)) \;+\; a_r\frac{x^r}{r!}. \tag{39}$$

Suppose the $C_r(x)$ satisfies $e^xC_r(x)=C_r(-x)$. Then, by considering the Laplace transform, the recursion (39) can be rewritten as

$$\widehat{C}_r(-z) \;=\; \sum_{n=0}^{r-1}\frac{(-z)^n}{n!}\widehat{C}_{r-n}(z) \;+\; a_r z^r. \tag{40}$$

Recall that, for a power series $C(x)=\sum_{m=0}^{\infty}c_m\frac{x^m}{m!}$, we denote by $\widehat{C}(z)=\sum_{m=0}^{\infty}c_m z^m$ its Laplace transform. In terms of the generating functions $C(z,t)=\sum_{r=1}^{\infty}\widehat{C}_r(z)t^r$ and $A(z)=\sum_{r=1}^{\infty}a_r z^r$, this is equivalent (since $\widehat{I^nC}(z)=z^n\widehat{C}(z)$) to the identity

$$C(-z,t) \;=\; e^{-zt}C(z,t) \;+\; A(zt). \tag{41}$$

In particular, $e^{z/2}A(z)$ must be an odd power series. Conversely, we can show that if this oddness property holds for $A(z)$, the power series $C_r(x)$ have the desired property $e^xC_r(x)=C_r(-x)$. The following lemma shows that $a_r=\frac{(-1)^r\binom{r-1}{2\nu}}{(r+2\nu)!}$ satisfies this property for all $\nu\ge 0$.

Lemma 1. *For all $\nu\ge 0$, we have*

$$e^{-z/2}\sum_{r=1}^{\infty}\frac{\binom{r-1}{2\nu}}{(r+2\nu)!}z^r \;=\; \frac{z}{(2\nu)!}\,\widehat{I}_\nu\Big(\frac{z}{2}\Big),$$

where $\widehat{I}_\nu(z)$ is the renormalized I-Bessel function of index $2\nu+\frac12$ and is given explicitly by

$$\widehat{I}_\nu(z) \;=\; \sum_{s=\nu}^{\infty}\frac{z^{2s}}{2^{s-\nu}(s-\nu)!\,(2s+2\nu+1)!!} \;=\; z^{2\nu}\Big(\frac{1}{z}\frac{d}{dz}\Big)^{2\nu}\frac{\sinh z}{z}.$$

Proof. Both sides satisfy the same differential equation and start with $\frac{z^{2\nu+1}}{(4\nu+1)!}$. $\square$

Remark. The second identity for $\widehat{I}_\nu(z)$ is Rayleigh's formula. The first few examples are:

$$\begin{aligned}
\widehat{I}_0(z) &= \frac{\sinh z}{z} = 1+\frac{z^2}{6}+\frac{z^4}{120}+\frac{z^6}{5040}+\frac{z^8}{362880}+\frac{z^{10}}{39916800}+\cdots,\\
\widehat{I}_1(z) &= \Big(1+\frac{3}{z^2}\Big)\frac{\sinh z}{z}-3\frac{\cosh z}{z^2} = \frac{z^2}{15}+\frac{z^4}{210}+\frac{z^6}{7560}+\frac{z^8}{498960}+\cdots,\\
\widehat{I}_2(z) &= \Big(1+\frac{45}{z^2}+\frac{105}{z^4}\Big)\frac{\sinh z}{z}-\Big(10+\frac{105}{z^2}\Big)\frac{\cosh z}{z^2} = \frac{z^4}{945}+\frac{z^6}{20790}+\cdots
\end{aligned}$$

We now define a set of elements $\{X_\nu^{(k)}\mid 0\le\nu<k/2\}$ of $\mathfrak{V}_k$ by

$$X_\nu^{(k)} \;=\; \sum_{\nu\le i<k/2}\frac{2^{\nu-3i}}{(i-\nu)!\,(2i+2\nu+1)!!}\,U_{k-2i}^{(k)}\,. \tag{42}$$

Here and in the following, $U_m^{(k)}$ denotes the weight k part of $U(k,m)$, which we only use for $m\le k$. This is equal to $U(k,m)$ if $0<m<k$, but $U_k^{(k)}$ is different from $U(k,k)$, and can be expressed by the basis elements by taking the weight k part of (30) for $j=k$, in which case the left-hand side is 0, as

$$U_k^{(k)} \;=\; -\sum_{\substack{0<m<k\\ m\equiv k(2)}}\frac{2^{m-k}}{(k-m)!}\,U_m^{(k)}\,. \tag{43}$$

Also we set $X_0^{(0)}=-1$ and $X_\nu^{(0)}=0$ if $\nu>0$. Here are examples of $X_\nu^{(k)}$ for small ν:

$$\begin{aligned}
X_0^{(k)} &= U_k^{(k)} + \frac{1}{24}U_{k-2}^{(k)} + \frac{1}{1920}U_{k-4}^{(k)} + \frac{1}{322560}U_{k-6}^{(k)} + \frac{1}{92897280}U_{k-8}^{(k)} + \cdots \\
&= -\frac{1}{12}\left(U_{k-2}^{(k)} + \frac{1}{40}U_{k-4}^{(k)} + \frac{1}{4480}U_{k-6}^{(k)} + \frac{1}{967680}U_{k-8}^{(k)} + \cdots\right), \\
X_1^{(k)} &= \frac{1}{60}\left(U_{k-2}^{(k)} + \frac{1}{56}U_{k-4}^{(k)} + \frac{1}{8064}U_{k-6}^{(k)} + \frac{1}{2128896}U_{k-8}^{(k)} + \cdots\right), \\
X_2^{(k)} &= \frac{1}{15120}\left(U_{k-4}^{(k)} + \frac{1}{88}U_{k-6}^{(k)} + \frac{1}{18304}U_{k-8}^{(k)} + \frac{1}{6589440}U_{k-10}^{(k)} + \cdots\right), \\
X_3^{(k)} &= \frac{1}{8648640}\left(U_{k-6}^{(k)} + \frac{1}{120}U_{k-8}^{(k)} + \frac{1}{32640}U_{k-10}^{(k)} + \cdots\right).
\end{aligned}$$

Note that the identity

$$\sum_{0\le\nu<k/2}(4\nu+1)X_\nu^{(k)} = 0 \tag{44}$$

holds. This can be seen from equation (43) and the definition (42) by comparing the coefficients of $U_{k-2i}^{(k)}$ for each i, which reduces to the specialization $x=2i+1/2$ of the identity (easily proved by induction) $\sum_{l=0}^{i}(x-2l)\binom{x}{l}=x\binom{x-1}{i}$. Hence, the coefficients $B_{r,\nu}(x)$ in (36) should be unique if the formula (36) holds true for all j and k because the first coefficient $B_{r,0}(x)$ is forced to be $-\mathcal{V}_r^{(0)}(x)/r!$ since $X_0^{(0)}=-1$ and $X_\nu^{(0)}=0$ for $\nu>0$.

We finally prove (36). When $k=0$ $(r=j)$, the right-hand side becomes $-B_{j,0}(x)$ as just mentioned. On the other hand, by taking the weight 0 part of the identity (22), we obtain the recursion

$$(e^x-1)\frac{\mathcal{V}_j^{(0)}(x)}{j!} = \sum_{n=1}^{j}\frac{(-1)^n}{n!}I^n\left(\frac{\mathcal{V}_{j-n}^{(0)}(x)}{(j-n)!}\right).$$

This is the same recursion as the one for $B_{j,0}(x)$ because $I^j(\mathcal{V}_0^{(0)}(x))=x^j/j!$. Since we know from (24) that $\mathcal{V}_1^{(0)}(x)=x/(e^x-1)=-B_{1,0}(x)$, we proved that (36) holds for $k=0$. Similarly, when $1\le k<j$, we take the weight k part of (22) to obtain

$$(e^x-1)\mathcal{V}_j^{(k)}(x) = \sum_{n=1}^{j-k-1}(-1)^n\binom{j}{n}I^n\big(\mathcal{V}_{j-n}^{(k)}(x)\big) + \sum_{\ell=1}^{k}(-1)^\ell\binom{j}{k-\ell}V(-\ell,k-\ell)\frac{(-x)^{j-k}}{(j-k)!}.$$

Using this, we can show that the both sides of (36) satisfy the same recursion, if we could show the identity

$$\sum_{\ell=1}^{k}(-1)^\ell\frac{V(-\ell,k-\ell)}{(r+\ell)!(k-\ell)!} = (r-1)!\sum_{0\le\nu<r/2}\frac{4\nu+1}{(r+2\nu)!(r-1-2\nu)!}X_\nu^{(k)}, \tag{45}$$

where $r=j-k$. By writing $V(-\ell,k-\ell)$ and $X_\nu^{(k)}$ in terms of $U_m^{(k)}$ using (30) and (42), and looking at the coefficients of $U_{k-2i}^{(k)}$ $(0<i<k/2)$ on both sides, this boils down (after some simple manipulations) to the binomial identity

$$\sum_{\ell=0}^{m}(-2)^{m-\ell}\binom{x}{\ell} = \sum_{\substack{n=0\\ n\equiv m(2)}}^{m}\frac{2n+1}{2^{n+1}(n+1)}\binom{\frac{m+n+1}{2}}{n+1}^{-1}\binom{x}{m-n}\binom{x-m-1}{n}. \tag{46}$$

To prove this, we note the obvious recursion satisfied by the left-hand side $L(m)$:

$$L(m) + 2\,L(m-1) \;=\; \binom{x}{m}.$$

If we can show the right-hand side of (46) (=: $R(m)$) satisfies the same recursion, we are done by induction on m (the initial condition is $L(0) = R(0) = 1$, which trivially holds). Denote the nth term of $R(m)$ by $R(m,n)$ and set $R_1(m,n) = R(m,n) + 2R(m-1,n-1)$ ($R(m-1,-1) = 0$). We have the identity

$$R_1(m,n) \;=\; \frac{m-n+2}{2n-3}\,R(m,n-2) \;-\; \frac{m-n}{2n+1}\,R(m,n) \tag{47}$$

because if we divide both sides by $R(m,n)/(2n+1)$, this becomes the trivial identity

$$2n+1 \,+\, \frac{2(2n-1)(m+n+1)(x-m)}{(x-m-n+1)(x-m-n)} \;=\; \frac{(m+n+1)(x-m+n)(x-m+n-1)}{(x-m-n+1)(x-m-n)} \,-\, m+n\,.$$

By summing (47) over $n \equiv m \pmod 2$ and telescoping, we complete the proof. □

3. Special identities among $\mathcal{A}$-multiple zeta values

Using the algorithms explained in §1 and below, we conducted numerical experiments (using Pari-GP) and conjectured several identities among finite multiple zeta values, which we will present in this section in a somewhat random order. A number of them were also found by other people and/or have been proved in the interim, and this will be mentioned as appropriate.

We first say a few words about the rapid calculation of $\mathcal{A}$MZVs. At the end of §1 we already discussed how to find $\mathbb{Q}$-linear relations among numbers in the ring $\mathcal{A}$ if these are known "to high precision," i.e., if we have their p-components for a fairly large number of primes p. These individual primes used do not need to be very large, since if we use all primes even in some quite modest interval $A < p < B$, like $A = 30$, $B = 300$, then the number $P = \prod_{A<p<B} p$ is still very large and experimentally discoverd congruences modulo P with reasonably small coefficients are extremely unlikely to be accidental. This still leaves the question of computing the individual mod p multiple zeta values. Using the definition (3) directly would be very slow, since it contains $\mathrm{O}(p^r)$ terms. However, there is a very easy algorithm that computes $\zeta_p(k_1,\ldots,k_r)$ in only $\mathrm{O}(pr)$ steps. If we recall that (3) defines $\zeta_M(k_1,\ldots,k_r) \in \mathbb{Q}$ for any $M \in \mathbb{N}$, not just for primes, then we have the obvious recursion

$$\zeta_{M+1}(k_1,\ldots,k_s) \;=\; \zeta_M(k_1,\ldots,k_s) \,+\, \frac{1}{M^{k_s}}\,\zeta_M(k_1,\ldots,k_{s-1})$$

for any M and s. Applying this with $M = 1,\ldots,p-1$ and $s = 1,\ldots,r$ (where we must interpret $\zeta_M(k_1,\ldots,k_{s-1})$ as 1 in the case $s = 1$), we get a recursion that allows us to compute each of these numbers from its predecessors by a single multiplication and a single addition, resulting in an $\mathrm{O}(pr)$ algorithm for $\zeta_p(k_1,\ldots,k_r)$ as claimed. Of course in doing this calculation we do all computations in $\mathbb{Z}/pZ$, not in $\mathbb{Q}$.

a. $\mathcal{A}$MZVs of low weight; dimension conjecture. The most striking property of the classical multiple zeta values (1) is that they satisfy so many linear relations over $\mathbb{Q}$, e.g., that of the 1024 MZVs of weight 12, only 12 (more precisely: at most 12) are linearly independent. As we already said in the introduction, the same phenomenon happens also for the $\mathcal{A}$-multiple zeta values and we again find many linear dependencies over $\mathbb{Q}$, a typical case being equation (7). More precisely, using the numerical algorithms just described to compute all $\mathcal{A}$MZVs of weight up to 16 and many up to weight 20, we were led to the conjecture (6). Recall that the basic conjectural statement stated in the introduction, says that the ring of $\mathcal{A}$MZVs is isomorphic to the quotient of the ring of usual MZVs by the ideal generated by π^2, and that this gives the conjectural dimension formula (6). Here is a complete list of the conjectural multiplicative generators of $\mathfrak{Z}_{\mathcal{A}}$ up to weight 16:

1. $Z_{\mathcal{A}}(3)$, $Z_{\mathcal{A}}(5)$, $Z_{\mathcal{A}}(7)$, $Z_{\mathcal{A}}(9)$, $Z_{\mathcal{A}}(11)$, $Z_{\mathcal{A}}(13)$, $Z_{\mathcal{A}}(15)$.
2. $\zeta_{\mathcal{A}}(1,1,6)$, $\zeta_{\mathcal{A}}(1,1,8)$, $\zeta_{\mathcal{A}}(1,1,10)$, $\zeta_{\mathcal{A}}(1,1,12)$, $\zeta_{\mathcal{A}}(1,3,10)$, $\zeta_{\mathcal{A}}(1,1,14)$, $\zeta_{\mathcal{A}}(1,3,12)$.
3. $\zeta_{\mathcal{A}}(1,1,1,8)$, $\zeta_{\mathcal{A}}(1,1,1,10)$, $\zeta_{\mathcal{A}}(1,1,2,9)$, $\zeta_{\mathcal{A}}(1,1,1,12)$, $\zeta_{\mathcal{A}}(1,1,2,11)$.
4. $\zeta_{\mathcal{A}}(1,1,1,1,8)$, $\zeta_{\mathcal{A}}(1,1,1,1,10)$, $\zeta_{\mathcal{A}}(1,1,1,1,12)$, $\zeta_{\mathcal{A}}(1,1,1,3,10)$, $\zeta_{\mathcal{A}}(1,1,1,4,9)$.
5. $\zeta_{\mathcal{A}}(1,1,1,1,1,10)$.

Finally, we also recall here the Broadhurst-Kreimer conjecture. Define $d_{k,n} = \dim(\mathfrak{Z}_k^n/\mathfrak{Z}_k^{(n-1)})$ = "number of $\mathbb{Q}$-linearly independent MZVs of weight k and depth exactly n". Then the B-K conjecture is the generating function identity

$$\sum_{k,n} d_{k,n}\, x^k y^n \ \stackrel{?}{=}\ \frac{1+\mathcal{E}y}{1-\mathcal{O}y+\mathcal{S}(y^2-y^4)}\,,$$

where $\mathcal{E} = x^2 + x^4 + \cdots = \frac{x^2}{1-x^2}$ and $\mathcal{O} = x^3 + x^5 + \cdots = \frac{x^3}{1-x^2}$ correspond to the even and odd simple zeta values, respectively, and $\mathcal{S} = \sum_{k\ge 0} \dim S_k(\mathrm{SL}_2(\mathbb{Z}))x^k = \frac{x^{12}}{(1-x^4)(1-x^6)}$ is the Hilbert-Poincaré series of cusp forms. The corresponding formula for the numbers $d_{k,n}^{\mathrm{red}}$ giving the dimensions of the associated bigraded pieces of $\mathfrak{Z}^{\mathrm{red}} = \mathfrak{Z}/\pi^2\mathfrak{Z}$ is then

$$\sum_{k,n} d_{k,n}^{\mathrm{red}}\, x^k y^n \ \stackrel{?}{=}\ \frac{1}{1-\mathcal{O}y+\mathcal{S}(y^2-y^4)}\,,$$

which reduces to (6) if we set $y=1$.

b. $\mathcal{A}$MZVs of small depth

We already saw in Example 7 of §1 that the finite single zeta values $\zeta_{\mathcal{A}}(k)$ all vanish. The next case is that of double zeta values. Here a simple calculation that will be discussed and generalized in the next section gives the formula

$$\zeta_{\mathcal{A}}(a,b) \ = \ \begin{cases} 0 & \text{if } k=a+b \text{ is even,} \\ (-1)^b\binom{k}{b}\, Z_{\mathcal{A}}(k) & \text{if } k \text{ is odd,} \end{cases} \tag{48}$$

where $Z_{\mathcal{A}}(k) \in \mathcal{A}$ are the numbers defined in (11). For triple zeta values we have the formula

$$2\,\zeta_{\mathcal{A}}(a,b,c) \ = \ -\,\zeta_{\mathcal{A}}(a,b+c) \ - \ \zeta_{\mathcal{A}}(a+b,c) \qquad \text{for } k=a+b+c \text{ odd,} \tag{49}$$

where the right-hand side can also be written as an integer multiple of $Z_{\mathcal{A}}(k)$ by (48). The first line of (48) and the formula (49) are special cases of the conjectural parity statement that any $\zeta_{\mathcal{A}}(k_1,\dots,k_r)$ with $k_1+\cdots+k_r \equiv r \pmod 2$ can be written as a linear combination of $\mathcal{A}$MZVs of shorter length. Unfortunately, we can prove only a weaker version of this. See Proposition 6 in §6.

Finally, there is a very interesting connection between triple $\mathcal{A}$MZVs of *even* weight—so those that cannot be reduced to double $\mathcal{A}$MZVs by the parity statement—and modular forms. Specifically, we experimentally found some concrete relations among triple $\mathcal{A}$MZVs, given in **g.** below. This also gives one more supporting piece of evidence for the definition given in the introduction (Main Conjecture) of the depth of an $\mathcal{A}$MZV as one less than the length of the argument, because for classical (real) MZVs there is a close link between *double* multiple zeta values and period polynomials of modular forms [13].

c. The sum formula and its variants. Recall the classical sum formula (conjectured by Hoffman and proved independently by Granville and by the second author), saying that the sum of $\zeta(\mathbf{k})$ for all admissible $\mathbf{k}$ of fixed weight k and depth (=length) r is equal to $\zeta(k)$. The corresponding statement for finite multiple zeta values is that, for any k and r, we have

$$\sum_{\substack{k_1+\cdots+k_r=k \\ k_r\geq 2}} \zeta_{\mathcal{A}}(k_1,\ldots,k_r) \;=\; \left(1+(-1)^r\binom{k-1}{r-1}\right) Z_{\mathcal{A}}(k)\,. \tag{50}$$

Note that without the restriction $k_r \geq 2$ the sum on the left is symmetric in the indices and becomes zero. This formula has now been proved by S. Saito and N. Wakabayashi [43] in a slightly generalized form (putting the condition $k_i \geq 2$ for any single i instead of $k_r \geq 2$).

Generalizing the sum formula, it was shown in [35] that the sum of all classical MZVs $\zeta(\mathbf{k})$ with $\mathbf{k} \in I(k,r,s)$ is a polynomial in Riemann zeta values, where $I(k,r,s)$ is the set of admissible indices $\mathbf{k}$ of weight k, depth r, and height (= number of components greater than 1) s. We did not find a corresponding statement for the $\mathcal{A}$MZVs, but we did find the conjectural identity

$$\sum_{r=1}^{k-1}(-1)^r \sum_{\mathbf{k}\in I(k,r,s)} \zeta_{\mathcal{A}}(\mathbf{k}) \;\overset{?}{=}\; 2\binom{k-1}{2s-1}\left(1-2^{1-k}\right) Z_{\mathcal{A}}(k)\,, \tag{51}$$

which can be regarded as an analogue of Le-Murakami's relation ([30, eq. (2)]). The identity (51) and a similar analogue of "Aoki-Ohno" formula were then proved in [24].

d. Hoffman duality. As noted in the introduction, the symmetric relation

$$\zeta_{\mathcal{A}}(k_1,\ldots,k_r) \;=\; (-1)^k \zeta_{\mathcal{A}}(k_r,\ldots,k_1) \tag{52}$$

holds trivially, where k is the weight. A less obvious duality was found by Hoffman. Its most natural expression ([14, Theorem 4.6]) uses the "star" (or "Euler") version of the $\mathcal{A}$MZVs in which the inequality sign $<$ in (3) is replaced by $\leq$, but he also gave a non-starred version ([14, Theorem 4.7]) which we can express in our terminology as

$$\zeta_{\mathcal{A}}(\mathbf{k}) \;=\; (-1)^r \sum_{\mathbf{k}'\succeq \mathbf{k}} \zeta_{\mathcal{A}}(\mathbf{k}')\,. \tag{53}$$

Here the relation $\mathbf{k}' \succeq \mathbf{k}$ means that the index $\mathbf{k}$ is obtained from $\mathbf{k}' = (k_1',\ldots,k_s')$ by replacing some of the commas by plus signs, e.g. $(1,3,2,1) \succeq (1+3,2+1) = (4,3)$.

We also found other $\mathcal{A}$MZV relations involving Hoffman's duality, like an $\mathcal{A}$-analogue of Ohno's relation ([34, Theorem 1]), whose statement we omit, that was proved in a special case by Yosuke Ihara and in general by Oyama [36] using the shuffle relation explained below.

e. $\mathcal{A}$MZVs with repeated arguments. Classical MZVs with repeated arguments are easy to evaluate by the simple formula

$$1 + \sum_{r=1}^{\infty} \zeta(\underbrace{k,k,\ldots,k}_{r})\, x^r \;=\; \exp\left(\sum_{n=1}^{\infty}(-1)^{n-1}\frac{\zeta(kn)}{n}x^n\right). \tag{54}$$

The obvious analogue in the $\mathcal{A}$-world is uninteresting. (It is true but both sides are equal to 1.) A non-trivial conjectural A-version of the case $k=3$ of (54) is given by

$$\sum_{r=0}^{\infty} \zeta_{\mathcal{A}}(\underbrace{1,2,1,2,\ldots,1,2}_{2r})\, x^r \overset{?}{=} \exp\biggl(\sum_{\substack{n=1\\ n \text{ odd}}}^{\infty} \zeta_{\mathcal{A}}(1,3n-1)\,\frac{x^n}{n^2}\biggr)\,. \tag{55}$$

In a different direction, for classical MZVs it was conjectured by the second author, and proved by Broadhurst and others [6], that

$$\zeta(\underbrace{1,3,\ldots,1,3}_{2r}) \;=\; \frac{2\pi^{4r}}{(4r+2)!}$$

for the classical multiple zeta values. Since $\pi^2=0$ in $\mathcal{A}$, the $\mathcal{A}$-analogue of this would naturally be

$$\zeta_{\mathcal{A}}(\underbrace{1,3,\ldots,1,3}_{2r}) \;=\; 0.$$

This is a special case of an identity proved by J. Zhao [52, Theorem 3.18], which has been further generalized by S. Saito and N. Wakabayashi [44].

Finally, as an analogue of an identity proved by the second author [51], we conjectured

$$\zeta_{\mathcal{A}}(\underbrace{2,\ldots,2}_{a},3,\underbrace{2,\ldots,2}_{b}) \;=\; 2\,(-1)^{a+b}\bigl(\zeta_{\mathcal{A}}(2a+1,2b+2)+\zeta_{\mathcal{A}}(2a+2,2b+1)\bigr)$$

and

$$\zeta_{\mathcal{A}}(\underbrace{2,\ldots,2}_{a},1,\underbrace{2,\ldots,2}_{b}) \;=\; 2\,(-1)^{a+b+1}\bigl(1-2^{1-k}\bigr)\,\bigl(\zeta_{\mathcal{A}}(2a,2b+1)+\zeta_{\mathcal{A}}(2a+1,2b)\bigr)$$

for any a, $b\ge 0$. (Of course, by (48) we can rewrite the right-hand sides of both formulas as simple multiples of $Z_{\mathcal{A}}(k)$, where k is the total weight $2a+2b+3$ resp. $2a+2b+1$.) These formulas were independently discovered and proved by Hessami Pilehrood et al. ([38, Theorems 4.1 and 4.2]).

There are a lot more specific linear relations known for classical multiple zeta values, examples being the cyclic sum formula [16], the derivation relation [17], the Bowman-Bradley relation [5] and so on. Attempts of finding $\mathcal{A}$-analogues of various relations have been made by many authors. For instance, analogues of those relations mentioned above were found and proved respectively by Kawasaki-Oyama [26], Murahara [33], and Saito-Wakabayashi [44]. For many more, we refer the reader to the web page [15] compiled by Hoffman.

f. Relation to multi-poly-Bernoulli numbers. The "modified poly-Bernoulli numbers" were already defined (equation (26)) in §2 in connection with harmonic moment sums, but they have other relations to finite multiple zeta values. For example, a result of Hoffman's ([14, Theorem 5.4]) can be stated in terms of these numbers and in our setting as

$$\zeta_{\mathcal{A}}(\underbrace{1,\ldots,1}_{j-1},i) \;=\; \bigl((-1)^{i+j}C^{(i-1)}_{p-1-j} \mod p\bigr)_p\,. \tag{56}$$

In fact, it turns out that this statement can be generalized to express all finite multiple zeta values in terms of appropriate "multi-poly-Bernoulli numbers". See [18, Theorem 8] for the precise statement. Note that (56) includes the formula $\zeta_{\mathcal{A}}(\underbrace{1,\ldots,1}_{k-2},2) = k\,Z_{\mathcal{A}}(k)$, since $C_n^{(1)}$ coincides with the nth Bernoulli number.

g. Relation to modular forms. Our last topic again concerns $\mathcal{A}$MZVs of low depth, but a different aspect of them. In the classical case, depth 2 even weight MZVs have an intriguing connection to the space of cusp forms on the modular group $\mathrm{SL}_2(\mathbb{Z})$ (see [13] for details), so it is now reasonable to look for a connection between *triple* $\mathcal{A}$MZVs and cusp forms of the same weight. We checked numerically up to weight 24 that the dimension of the space spanned by the triple multiple zeta values of even weight k is equal to $k/2-2-\dim S_k$, where S_k is the space of cusp forms of weight k on $\mathrm{SL}_2(\mathbb{Z})$. (Those of odd weight $k>1$ are always multiples of $Z_{\mathcal{A}}(k)$, as was mentioned in **b**.)

Moreover, we also experimentally discovered that the $\zeta_{\mathcal{A}}(1,n,k-1-n)$ with $0<n<k-1$ span the space of all triple $\mathcal{A}$MZVs of weight k and the following relations among them hold. Fix an even integer $k\geq 4$. Then for every even integer $2l\geq k/3$, we have the relation

$$\sum_{j=1}^{k-2} a_{2l-j}\,\zeta_{\mathcal{A}}(1,j,k-1-j) \;=\; 0, \tag{57}$$

of triple $\mathcal{A}$MZVs of weight k, where the numbers $a_n=a_n(k,l)$ are the coefficients of the expansion

$$\frac{(1-x+x^2)^{3l-k/2}}{(1-x)^{2l}} \;=\; a_0+a_1x+a_2x^2+\cdots,$$

with $a_n=0$ for $n<0$. These coefficients are given explicitly in terms of the "trinomial coefficients" $T(b,i)$, defined as the coefficient of x^i in $(1+x+x^2)^b$, and binomial coefficients by

$$a_n(k,l) \;=\; (-1)^n\sum_{m=0}^{n}\binom{-2l}{m}T(3l-k/2,n-m).$$

Equation (57) gives an infinite family of relations but of course only finitely many of them can be independent, and we found the number of independent relations is $[\frac{k}{3}]$. This looks not enough to give the dimension of cusp forms. However, we make the following refined conjecture, also based on the numerical data.

Conjecture 1. *Let k be an even integer. Then*

(1) *The elements $\zeta_{\mathcal{A}}(1,n,k-1-n)$ with $0<n<k/2-1$ span the space of all triple $\mathcal{A}$MZVs.*
(2) *Among these spanning elements, the relations (57) with $k/6\leq l<k/6+\dim S_k$ hold.*

We note that the interval in (2) automatically contains exactly $\dim S_k$ integers l, and that for such an l, the coefficients a_{2l-n} in (57) are zero if $n>k/2-2$. Moreover, we can show by the exact formula of a_n above that these $\dim S_k$ relations are independent. Hence, if the conjecture is true, the dimension of the space of triple $\mathcal{A}$MZVs is bounded above by $k/2-2-\dim S_k$.

We also checked up to weight 24 that the $\mathcal{A}$MZVs of the form $\zeta_{\mathcal{A}}(1,a,1,b)$ with a and b even span the same space as the triple $\mathcal{A}$MZVs. Note that the indices of this form with $a+b=k$ is $k/2-2$, and also that in the classical case the values $\zeta(a,b)$ with a,b odd span the double zeta space of even weight and we have as many linear relations among them as the dimension of S_k. A typical example of the relations that we found empirically is

$$\begin{aligned}&327\,\zeta_{\mathcal{A}}(1,2,1,12)\;+\;111\,\zeta_{\mathcal{A}}(1,4,1,10)\;+\;53\,\zeta_{\mathcal{A}}(1,6,1,8)\\&+59\,\zeta_{\mathcal{A}}(1,8,1,6)\;+\;120\,\zeta_{\mathcal{A}}(1,10,1,4)\;+\;366\,\zeta_{\mathcal{A}}(1,12,1,2)\;=\;0\end{aligned}$$

in weight 16 (where it is unique, since S_{16} is 1-dimensional). Note that this relation, and any other specific one, can be (and in this case has been) proved by using the shuffle relations that will be discussed in §7.

4. Multiple Seki-Bernoulli sums

We already saw that the finite single zeta values $\zeta_{\mathcal{A}}(a)$ all vanish, and mentioned in **b.** in the last section that the next case of double zeta values is given by the formula

$$\zeta_{\mathcal{A}}(a,b) \;=\; (-1)^b \binom{a+b}{b} Z_{\mathcal{A}}(a+b) \qquad (\,\forall\, a,\, b>0\,) \tag{58}$$

expressing the finite double zeta values in terms of the numbers $Z_{\mathcal{A}}(k) \in \mathcal{A}$ defined in (11). Indeed, we can use Fermat's little theorem and the Seki-Bernoulli formula for sums of powers of integers in terms of Bernoulli polynomials and Bernoulli numbers to write

$$\sum_{0<m<n} \frac{1}{m^a} \;\equiv\; \sum_{0<m<n} m^{p-1-a} \;=\; \frac{B_{p-a}(n)\,-\,B_{p-a}}{p-a} \;=\; \sum_{r=1}^{p-a} \frac{1}{p-a}\binom{p-a}{r} B_{p-a-r}\, n^r$$

for each sufficiently large prime p, where the congruence is taken modulo p. Now multiplying by n^{-b} and summing over $0<n<p$, and using that $\sum_{0<n<p} n^{r-b} \equiv -\delta_{r,b}$, we find

$$\zeta_{\mathcal{A}}(a,b)_{(p)} \;\equiv\; \sum_{0<m<n<p} \frac{1}{m^a n^b} \;\equiv\; -\frac{1}{p-a}\binom{p-a}{b} B_{p-a-b} \;\equiv\; (-1)^b \binom{a+b}{b} \frac{B_{p-a-b}}{a+b}\,,$$

which in view of the definition (11) of $Z_{\mathcal{A}}(k)$ is equivalent to (58). Equation (58) is also given, with substantially the same proof, by Hoffman [14, Theorem 6.1] and Zhao [52, Theorem 3.1], and the special case $a=1$, $b=k-1$ was already given by Vandiver [49, (63)]. Equation (58) implies in particular that the finite double zeta values $\zeta_{\mathcal{A}}(a,b)$ vanish whenever the weight $a+b$ is even. Conversely, those of odd weight should never vanish, according to the conjectural statement $Z_{\mathcal{A}}(k) \neq 0$ discussed in §1.

The same idea as was just used for the case of double zeta values shows that all $\zeta_{\mathcal{A}}(k_1,\dots,k_r)$ can be expressed in terms of "multiple Seki-Bernoulli sums," which we now define.

For $l \geq 0$ and $i \geq 1$, set

$$b(l,i) \;=\; -\frac{1}{l+1}\binom{l+1}{i} B_{l+1-i} \tag{59}$$

(with $B_n = 0$ if $n<0$), and for positive integers $k_1,\dots,k_r$ $(r \geq 2)$ define an element $\mathbb{B}(k_1,\dots,k_r)$ in $\mathcal{A}$ by

$$\mathbb{B}(k_1,\dots,k_r)_{(p)} \;=\; -\sum_{0=l_0 \leq l_1 \leq \cdots \leq l_{r-1}=p-k_r-1} \; \prod_{h=1}^{r-1} b(l_h, l_{h-1}+k_h)\,.$$

When $r=2$, the right-hand side is $-b(p-1-k_2,k_1) \equiv (-1)^{k_1-1}\binom{k_1+k_2}{k_1}\frac{B_{p-k_1-k_2}}{k_1+k_2}$ and we have

$$\mathbb{B}(k_1,k_2) \;=\; (-1)^{k_2}\binom{k_1+k_2}{k_1} Z_{\mathcal{A}}(k_1+k_2) \qquad (\;=\;\zeta_{\mathcal{A}}(k_1,k_2)\,)\,.$$

To express $\zeta_{\mathcal{A}}(\mathbf{k})$ in terms of $\mathbb{B}(\mathbf{k})$ by using the Seki-Bernoulli formula for sums of powers, it turns out that the "Euler version" of $\zeta_{\mathcal{A}}(\mathbf{k})$, i.e., the non-strict version (often referred to as the "zeta-star" value) $\zeta^\star_{\mathcal{A}}(\mathbf{k}) \;=\; \big(\zeta^\star_p(\mathbf{k}) \bmod p\big)_p$, where

$$\zeta^\star_p(k_1,\dots,k_r) \;=\; \sum_{0<n_1\le\cdots\le n_r<p} \frac{1}{n_1^{k_1}\cdots n_r^{k_r}}\,,$$

is easier to compute.

For $l \ge 0$, the Seki-Bernoulli formula can be written as

$$\sum_{0<m\le n} m^l \;=\; \sum_{i=1}^{l+1} (-1)^{l-i}\, b(l,i)\, n^i$$

with $b(l,i)$ as above. A convenient form we shall frequently use of this formula modulo a prime is the following. For $k, k' \ge 1$ and a large enough prime p, we have

$$\sum_{0<m\le n} m^{p-1-k} \;\equiv\; \sum_{i=1}^{k'-1} b(p-1-i,k)\, n^i + \sum_{l=k-1}^{p-1-k'} b(l,k)\, n^{p-1-l} \qquad (\mathrm{mod}\ p)\,. \tag{60}$$

Here, we have used $(-1)^{k+i} b(p-1-k,i) \;\equiv\; b(p-1-i,k)\ (\mathrm{mod}\ p)$.

To illustrate, let us compute $\zeta^\star_{\mathcal{A}}(k_1,k_2)_{(p)}$ and $\zeta^\star_{\mathcal{A}}(k_1,k_2,k_3)_{(p)}$ for p sufficiently large:

$$\begin{aligned}
\zeta^\star_{\mathcal{A}}(k_1,k_2)_{(p)} \;&\equiv\; \sum_{0<m_1\le m_2<p} m_1^{p-1-k_1} m_2^{-k_2} \\
&\equiv\; \sum_{0<m_2<p} \Bigg(\sum_{i=1}^{k_2-1} b(p-1-i,k_1)\, m_2^{i-k_2} + \sum_{l=k_1-1}^{p-1-k_2} b(l,k_1)\, m_2^{p-1-l-k_2} \Bigg) \\
&\equiv\; \sum_{i=1}^{k_2-1} b(p-1-i,k_1)\, \zeta_{\mathcal{A}}(k_2-i)_{(p)} + \sum_{l=k_1-1}^{p-1-k_2} b(l,k_1) \sum_{0<m_2<p} m_2^{p-1-l-k_2} \\
&\equiv\; -b(p-1-k_2,k_1) \quad (\mathrm{mod}\ p) \\
&=\; \mathbb{B}(k_1,k_2)_{(p)}
\end{aligned} \tag{61}$$

(where we have used $\zeta_{\mathcal{A}}(k_2-i)_{(p)} = 0$ for p and $\sum_{0<m_2<p} m_2^{p-1-l-k_2} \equiv 0$ except for $l = p-1-k_2$),

$$\begin{aligned}
&\zeta^\star_{\mathcal{A}}(k_1,k_2,k_3)_{(p)} \\
&\quad\equiv\; \sum_{0<m_1\le m_2\le m_3<p} m_1^{p-1-k_1} m_2^{-k_2} m_3^{-k_3} \\
&\quad\equiv\; \sum_{0<m_2\le m_3<p} \Bigg(\sum_{i=1}^{k_2-1} b(p-1-i,k_1)\, m_2^{i-k_2} m_3^{-k_3} + \sum_{l_1=k_1-1}^{p-1-k_2} b(l_1,k_1)\, m_2^{p-1-l_1-k_2} m_3^{-k_3} \Bigg) \\
&\quad\equiv\; -\sum_{i=1}^{k_2-1} \mathbb{B}(k_1,i)\zeta^\star_{\mathcal{A}}(k_2-i,k_3)_{(p)} \\
&\qquad + \sum_{l_1=k_1-1}^{p-1-k_2} b(l_1,k_1) \sum_{0<m_3<p} \Bigg(\sum_{i=1}^{k_3-1} b(p-1-i,l_1+k_2)\, m_3^{i-k_3} + \sum_{l_2=l_1+k_2-1}^{p-1-k_3} b(l_2,l_1+k_2)\, m_3^{p-1-l_2-k_3} \Bigg)
\end{aligned}$$

$$\begin{aligned}
&\equiv\; -\sum_{i=1}^{k_2-1}\mathbb{B}(k_1,i)\zeta^\star_{\mathcal{A}}(k_2-i,k_3)_{(p)} \;-\; \sum_{i=1}^{k_3-1}\mathbb{B}(k_1,k_2,i)\zeta^\star_{\mathcal{A}}(k_3-i)_{(p)}\\
&\quad +\sum_{l_1=k_1-1}^{p-1-k_2}\;\sum_{l_2=l_1+k_2-1}^{p-1-k_3} b(l_1,k_1)b(l_2,l_1+k_2)\sum_{0<m_3<p} m_3^{p-1-l_2-k_3}\\
&\equiv\; -\sum_{i=1}^{k_2-1}\mathbb{B}(k_1,i)\zeta^\star_{\mathcal{A}}(k_2-i,k_3)_{(p)}+\mathbb{B}(k_1,k_2,k_3)_{(p)}\,.
\end{aligned}$$

(Recall that $b(m,n)=0$ if $m<n-1$.) Continuing in the same way, we obtain the following proposition.

Proposition 3. *For any $r\ge 2$ and positive integers k_i $(1\le i\le r)$, we have*

$$\begin{aligned}
&\zeta^\star_{\mathcal{A}}(k_1,\dots,k_r)\\
&= -\sum_{i=1}^{k_2-1}\mathbb{B}(k_1,i)\zeta^\star_{\mathcal{A}}(k_2-i,k_3,\dots,k_r) \;-\; \sum_{i=1}^{k_3-1}\mathbb{B}(k_1,k_2,i)\zeta^\star_{\mathcal{A}}(k_3-i,k_4,\dots,k_r)\\
&\qquad -\;\cdots\cdots\;-\sum_{i=1}^{k_r-1}\mathbb{B}(k_1,\dots,k_{r-1},i)\zeta^\star_{\mathcal{A}}(k_r-i)\;+\;\mathbb{B}(k_1,\dots,k_r)\,.
\end{aligned}$$

Corollary 3. *We have $\mathbb{B}(k_1,\dots,k_r)\in\mathfrak{Z}_{\mathcal{A},k}$ $(k=k_1+\cdots+k_r)$.*

Proof. This can be seen by induction on the depth r, starting with $\mathbb{B}(k_1,k_2)=\zeta_{\mathcal{A}}(k_1,k_2)\in\mathfrak{Z}_{\mathcal{A},k_1+k_2}$. □

Corollary 4. *The $\mathbb{B}(k_1,\dots,k_r)$'s span the space $\mathfrak{Z}_{\mathcal{A}}$.*

Proof. The corollary follows from the proposition by induction, since the $\zeta^\star_{\mathcal{A}}(k_1,\dots,k_r)$ span the same space as the $\mathfrak{Z}_{\mathcal{A}}$ as the $\zeta_{\mathcal{A}}(k_1,\dots,k_r)$. □

The next corollary is equation (49) in §3.

Corollary 5 (Hoffman [14], Zhao [52])**.** *For $k=a+b+c$ odd, we have the formula*

$$2\,\zeta_{\mathcal{A}}(a,b,c)\;=\;-\,\zeta_{\mathcal{A}}(a,b+c)\;-\;\zeta_{\mathcal{A}}(a+b,c)$$

Proof. From the congruence above the proposition, we have

$$\zeta^\star_{\mathcal{A}}(a,b,c)\;=\;-\sum_{i=1}^{b-1}\mathbb{B}(a,i)\zeta_{\mathcal{A}}(b-i,c)+\mathbb{B}(a,b,c).$$

If the weight $a+b+c$ is odd, either $\mathbb{B}(a,i)=\zeta_{\mathcal{A}}(a,i)$ or $\zeta_{\mathcal{A}}(b-i,c)$ has even weight and hence vanishes, and thus

$$\zeta^\star_{\mathcal{A}}(a,b,c)\;=\;\zeta_{\mathcal{A}}(a,b,c)+\zeta_{\mathcal{A}}(a+b,c)+\zeta_{\mathcal{A}}(a,b+c)\;=\;\mathbb{B}(a,b,c)$$

in this case. By definition, the p-component of $\mathbb{B}(a,b,c)$ is

$$\mathbb{B}(a,b,c)_{(p)}\;=\;-\sum_{j=0}^{p-c-1} b(j,a)b(p-c-1,j+b).$$

Recalling that $b(m,n)$ is a multiple of the Bernoulli number B_{m+1-n}, and that the odd-index Bernoulli number vanishes except B_1, we see that the only non-zero terms on the right are for $j=a$ and $j=p-b-c-1$ because $(j+1-a)+(p-c-j-b)$ is odd. Hence we have

$$\begin{aligned}\mathbb{B}(a,b,c)_{(p)} &= -b(a,a)\,b(p-c-1,a+b)-b(p-b-c-1,a)\,b(p-c-1,p-c-1)\\ &= -\frac{1}{2}\left(b(p-c-1,a+b)+b(p-b-c-1,a)\right)\\ &= \frac{1}{2}\left(\zeta_{\mathcal{A}}(a+b,c)_{(p)}+\zeta_{\mathcal{A}}(a,b+c)_{(p)}\right)\end{aligned}$$

and obtain the desired formula. □

5. "True" zeta values: heuristic arguments and conjectural formulas

In a different direction, we can ask whether there is a natural definition of numbers $Z_{\mathcal{A}}(a,b)\in\mathcal{A}$ (or more generally $Z_{\mathcal{A}}(k_1,\dots,k_r)$) analogous to the definition of $Z_{\mathcal{A}}(k)$ in §1 that is a good analogue of classical double (or multiple) zeta values. Under our main conjecture, these should correspond to $\zeta(k_1,\dots,k_r)$ mod π^2 in $\mathfrak{Z}^{\mathrm{red}}=\mathfrak{Z}/(\pi^2)$.

Following the same idea of "backwards extrapolation" as was used in (11), where we argued that the $\mathcal{A}$-analogue of $\zeta(k)$ should be

$$\zeta(k)\ \text{“}\equiv\text{”}\ \sum_{0<m} m^{p-1-k} \;=\; \zeta(-p+1+k) \;=\; -\frac{B_{p-k}}{p-k} \;\equiv\; Z_{\mathcal{A}}(k)_{(p)}\,,$$

we compute in the depth 2 case (using (60)) as

$$\begin{aligned}\zeta^{\star}(a,b) &= \sum_{0<m\le n} m^{-a}n^{-b}\ \text{“}\equiv\text{”}\ \sum_{0<m\le n} m^{p-1-a}n^{-b}\\ &\equiv \sum_{0<n}\left(\sum_{i=1}^{b-1} b(p-1-i,a)\,n^{i-b}+\sum_{l=a-1}^{p-1-b} b(l,a)\,n^{p-1-l-b}\right)\\ &\text{“}=\text{”}\ \sum_{i=1}^{b-1} b(p-1-i,a)\,\zeta(b-i)\;+\;\sum_{l=a-1}^{p-1-b} b(l,a)\,\zeta(-p+1+l+b)\end{aligned}$$

with $b(l,a)$ as in (59). Based on this computation, we would like to be able to define an $\mathcal{A}$-analogue $Z_{\mathcal{A}}(a,b)$ of $\zeta(a,b)$ by

$$\begin{aligned}Z_{\mathcal{A}}(a,b) &= Z^{\star}_{\mathcal{A}}(a,b)-Z_{\mathcal{A}}(a+b)\\ &\text{“}=\text{”}\ -\sum_{i=1}^{b-1}(-1)^a\binom{a+i}{a}Z_{\mathcal{A}}(a+i)\,Z_{\mathcal{A}}(b-i)+\widetilde{\mathbb{B}}(a,b)\;-\;Z_{\mathcal{A}}(a+b)\,,\end{aligned}\tag{62}$$

where we have set $\widetilde{\mathbb{B}}(a,b)=\left(\widetilde{\mathbb{B}}(a,b)_{(p)} \bmod p\right)_p$ with

$$\widetilde{\mathbb{B}}(a,b)_{(p)} \;=\; \sum_{l=a-1}^{p-1-b} b(l,a)\,\zeta(-p+1+l+b)\ \left(\equiv\ -\sum_{l=a-1}^{p-1-b}\binom{l+1}{a}\frac{B_{l+1-a}}{l+1}\,\frac{B_{p-l-b}}{l+b} \bmod p\right).$$

(More generally, we define $\widetilde{\mathbb{B}}(k_1,\dots,k_r)=\big(\widetilde{\mathbb{B}}(k_1,\dots,k_r)_{(p)} \bmod p\big)_p$ with

$$\widetilde{\mathbb{B}}(k_1,\dots,k_r)_{(p)} \;=\; \sum_{0=l_0\le l_1\le\cdots\le l_{r-1}\le p-k_r-1}\;\prod_{h=1}^{r-1} b(l_h,l_{h-1}+k_h)\,\zeta(-p+l_{r-1}+k_r+1)\,.$$

Note that the previously defined $\mathbb{B}(k_1,\dots,k_r)$ can also be written in a parallel manner as

$$\mathbb{B}(k_1,\dots,k_r)_{(p)} \;=\; \sum_{0=l_0\le l_1\le\cdots\le l_{r-1}\le p-k_r-1}\;\prod_{h=1}^{r-1} b(l_h,l_{h-1}+k_h)\,\zeta_{\mathcal{A}}(-p+l_{r-1}+k_r+1)_{(p)}\,.)$$

The problem is that (62) contains the divergent expression $(-1)^a\binom{k-1}{a}Z_{\mathcal{A}}(k-1)Z_{\mathcal{A}}(1)$ ($k=a+b$), and we need to "regularize" this term to extract a finite quantity. We choose

$$(-1)^a\binom{k-1}{a}\Big((\gamma_{\mathcal{A}}-H_{k-1}+H_{b-1})\,Z_{\mathcal{A}}(k-1)\;-\;Z'_{\mathcal{A}}(k-1)\Big)$$

as a regularized value, where $\gamma_{\mathcal{A}}$ and $Z'_{\mathcal{A}}(k-1)$ are the $\mathcal{A}$-analogues of Euler's constant and of the derivative of ζ as defined in Examples 4 and 9 of §1. Our argument is as follows. Since

$$\binom{s-1}{a}' \;=\; \binom{s-1}{a}\big(\psi(s)\;-\;\psi(s-a)\big)\;\left(=\;\binom{s-1}{a}(H_{s-1}-H_{s-a-1})\text{ if } s\in\mathbb{N}\right),$$

($\psi(s)$ is the digamma function) we have the expansion near $\epsilon=0$

$$\begin{aligned}&\binom{k-\epsilon-1}{a}\zeta(k-\epsilon-1)\zeta(1+\epsilon)\\ &=\;\frac{\binom{k-1}{a}\zeta(k-1)}{\epsilon}\;+\;\binom{k-1}{a}\Big((\gamma-H_{k-1}+H_{k-a-1})\zeta(k-1)-\zeta'(k-1)\Big)\;+\;O(\epsilon)\,.\end{aligned}$$

So our choice of the regularized values is the "Kronecker limit" of $\binom{k-s}{a}\zeta(k-s)\zeta(s)$ at $s=1$. Based on this heuristic argument, we make the following definition.

Definition. *For $a,b\ge 1$ we define $Z_{\mathcal{A}}(a,b)\in\mathcal{A}$ by*

$$\begin{aligned}Z_{\mathcal{A}}(a,b)\;:=\;\widetilde{\mathbb{B}}(a,b)\;-\;&\sum_{i=1}^{b-2}(-1)^i\binom{a+i}{a}Z_{\mathcal{A}}(a+i)\,Z_{\mathcal{A}}(b-i)\;-\;Z_{\mathcal{A}}(k)\\ &+\;(-1)^a\binom{k-1}{a}(H_{b-1}-H_{k-1})\,Z_{\mathcal{A}}(k-1)+X_k\,,\end{aligned}\tag{63}$$

where $Z_{\mathcal{A}}(\,\cdot\,)$ is as in (11), $k=a+b$, and

$$X_k\;=\;(-1)^a\binom{k-1}{a}\big(\gamma_{\mathcal{A}}Z_{\mathcal{A}}(k-1)\;-\;Z'_{\mathcal{A}}(k-1)\big),$$

with $\gamma_{\mathcal{A}}$ and $Z'_{\mathcal{A}}$ as in (10) and (14).

This rather complicated definition turns out to work perfectly! What do we mean by that? Actually, several things:

i) The right-hand side of (63) should not just be in $\mathcal{A}$, but in $\mathfrak{Z}_{\mathcal{A}}$. We have verified this numerically in low weights (up to around 20). For $k=a+b$ odd, we can prove it, because a simple calculation using the properties of Bernoulli numbers and $Z_{\mathcal{A}}(k-1) = Z'_{\mathcal{A}}(k-1) = 0$ gives

$$Z_{\mathcal{A}}(a,b) \;=\; -\frac{1}{2}(1+(-1)^a\binom{k}{a})\,Z_{\mathcal{A}}(k)\,. \tag{64}$$

Note that this also agrees modulo π^2 with the formula (33) in [51] for real double zeta values of odd weight. For k even we do not have a proof, but experimentally we found the formula

$$(-1)^n\sum_{j=1}^{n}\binom{k-j}{k-n}Z_{\mathcal{A}}(j,k-j) \;=\; \zeta_{\mathcal{A}}(n-1,1,k-n) \,-\, Z_{\mathcal{A}}(n)\,Z_{\mathcal{A}}(k-n) \qquad (2\le n\le k-1),$$

and this (together with $Z_{\mathcal{A}}(1,k-1)+\sum_{j=1}^{k-1}Z_{\mathcal{A}}(j,k-j)=0$, which is also experimental) can be solved to give the closed formula.

$$Z_{\mathcal{A}}(i,k-i) \;=\; (-1)^i\sum_{n=2}^{k-1}\left(\binom{k-n}{k-i}-\frac{1}{2}\binom{k-1}{k-i}\right)\bigl(\zeta_{\mathcal{A}}(n-1,1,k-n)-Z_{\mathcal{A}}(n)\,Z_{\mathcal{A}}(k-n)\bigr) \tag{65}$$

for all even k and all $0<i<k$, where $Z_{\mathcal{A}}(1)$ is defined to be 0, in which all terms on the right-hand side belong to $\mathfrak{Z}_{\mathcal{A}}$. This formula is conjectural for the moment, but presumably could be proved with some effort.

ii) Furthermore, as well as belonging to $\mathfrak{Z}_{\mathcal{A}}$, the numbers defined by (63) satisfy all of the relations among ordinary double zeta values, as studied in detail in [13].

iii) Finally, these numbers coincide numerically up to weight 18 with the element in $\mathcal{A}$ which corresponds to $\zeta(a,b)$ under our "main conjecture" as stated in the introduction and discussed in detail in §8.

For "modular relations" of the double zeta values, by using (65), we can translate relations in [13] into those among $\zeta_{\mathcal{A}}(n-1,1,k-n)-Z_{\mathcal{A}}(n)Z_{\mathcal{A}}(k-n)$. But this is not satisfactory. What we want to obtain is a direct relationship between period polynomials and relations among $\zeta_{\mathcal{A}}(a,b,c)$s, and we have not yet succeeded to do so. What we have found experimentally was described in **g.** of §3.

Also, we expect that $Z_{\mathcal{A}}(n)\,Z_{\mathcal{A}}(k-n)$ can be written in terms of length 3 $\zeta_{\mathcal{A}}(a,b,c)$, since $Z_{\mathcal{A}}(n)\,Z_{\mathcal{A}}(k-n)$ should have depth 2. On this, we experimentally found the following. For even k and odd j with $1\le j\le k/2-2$, put

$$H_{k,j} \;:=\; \frac{1}{2}\sum_{n=j+2}^{k-j-2}\binom{n}{j}\binom{k-n}{j}Z_{\mathcal{A}}(n)\,Z_{\mathcal{A}}(k-n).$$

This can be solved in $Z_{\mathcal{A}}(n)\,Z_{\mathcal{A}}(k-n)$ with odd $n\ge 3$ since the coefficient matrix is upper triangular with non-zero diagonal entries (however, we have not found an explicit formula of the inverse matrix), and we also have the explicit conjectural formula

$$\begin{aligned} H_{k,j} \;&=\; (j+1)\,\zeta_{\mathcal{A}}(j+1,j,k-2j-1)+(k-2j-1)\,\zeta_{\mathcal{A}}(j,j,k-2j)\\ &\quad+(j+1)\,\zeta_{\mathcal{A}}(j,j+1,k-2j-1). \end{aligned}$$

For the case of depth 3, a similar heuristic argument suggests

$$\begin{aligned} Z_{\mathcal{A}}(a,b,c) \;\text{“}=\text{”}\; &\widetilde{\mathbb{B}}(a,b,c) \,-\, Z_{\mathcal{A}}(a+b,c) \,-\, Z_{\mathcal{A}}(a,b+c) \,-\, Z_{\mathcal{A}}(a+b+c)\\ &-\sum_{i=1}^{b-1}\zeta_{\mathcal{A}}(a,i)\bigl(Z_{\mathcal{A}}(b-i,c) \,+\, Z_{\mathcal{A}}(b+c-i)\bigr) \,-\, \sum_{i=1}^{c-1}\mathbb{B}(a,b,i)\,Z_{\mathcal{A}}(c-i)\,. \end{aligned} \tag{66}$$

As in the case of depth 2, we need to regularize the term $\mathbb{B}(a,b,c-1)Z_{\mathcal{A}}(1)$.

First, suppose the weight $k=a+b+c$ is even. In this case, $\mathbb{B}(a,b,c-1)$ is equal to

$$\frac{1}{2}\big(\zeta_{\mathcal{A}}(a,b+c-1)+\zeta_{\mathcal{A}}(a+b,c-1)\big) \;=\; \frac{1}{2}\Big((-1)^a\binom{k-1}{a} \;+\; (-1)^{a+b}\binom{k-1}{a+b}\Big)Z_{\mathcal{A}}(k-1)\,.$$

(See Corollary 5 of Proposition 3 in §4.) With this we may use the same regularization as before and define as follows (noting $Z_{\mathcal{A}}(k)=0$ when k is even).

Definition. *For $a,b,c\ge 1$ with $a+b+c$ even, set*

$$\begin{aligned}
Z_{\mathcal{A}}(a,b,c) \;:=\;& \widetilde{\mathbb{B}}(a,b,c) \;-\; Z_{\mathcal{A}}(a+b,c) \;-\; Z_{\mathcal{A}}(a,b+c)\\
&- \sum_{i=1}^{b-1}\zeta_{\mathcal{A}}(a,i)\big(Z_{\mathcal{A}}(b-i,c) \;+\; Z_{\mathcal{A}}(b+c-i)\big) \;-\; \sum_{i=1}^{c-2}\mathbb{B}(a,b,i)\,Z_{\mathcal{A}}(c-i)\\
&+ \frac{1}{2}(-1)^a\binom{k-1}{a}\big((\gamma_{\mathcal{A}}-H_{k-1} \;+\; H_{k-a-1})Z_{\mathcal{A}}(k-1) \;-\; Z'_{\mathcal{A}}(k-1)\big)\\
&+ \frac{1}{2}(-1)^c\binom{k-1}{c-1}\big((\gamma_{\mathcal{A}}-H_{k-1} \;+\; H_{c-1})Z_{\mathcal{A}}(k-1) \;-\; Z'_{\mathcal{A}}(k-1)\big)\,.
\end{aligned}$$

We have checked numerically up to weight 18 that this coincides with the predicted value. We should, however, note that this is very subtle. If we change $\binom{k-1}{a+b}Z_{\mathcal{A}}(k-1)Z_{\mathcal{A}}(1)$ into $\binom{k-1}{c-1}Z_{\mathcal{A}}(k-1)Z_{\mathcal{A}}(1)$ and then normalize in the same way as was done above, then the resulting $\binom{k-1}{c-1}\big((\gamma_{\mathcal{A}}-H_{k-1} \;+\; H_{a+b})Z_{\mathcal{A}}(k-1) \;-\; Z'_{\mathcal{A}}(k-1)\big)$ is different and does not give the correct value of $Z_{\mathcal{A}}(a,b,c)$!

As for the question whether this is in $\mathfrak{Z}_{\mathcal{A},k}$ ($k=a+b+c$), we found the following.

Conjecture 2. *Let $a,b,c\ge 1$ and assume $a+b+c$ is even. Then*

$$\begin{aligned}
Z_{\mathcal{A}}(a,b,c) \;=\;& -\frac{1}{2}\left(Z_{\mathcal{A}}(a+b,c)+Z_{\mathcal{A}}(a,b+c)\right)\\
&- \frac{(-1)^a}{2}\sum_{j=0}^{a}\binom{b+j-1}{j}\binom{a+c-j}{c}Z_{\mathcal{A}}(b+j,a+c-j)\\
&+ \frac{(-1)^b}{2}\sum_{j=1}^{b}\binom{a+j-1}{j}\binom{b+c-j}{c}Z_{\mathcal{A}}(a+j)\,Z_{\mathcal{A}}(b+c-j).
\end{aligned}$$

The odd weight case is more complicated. To regularize the term $\mathbb{B}(a,b,c-1)Z_{\mathcal{A}}(1)$ in (66), we start with the empirically discovered formula

$$\begin{aligned}
\mathbb{B}(a,b,c-1)\Big(=\;& \zeta_{\mathcal{A}}(a,b,c-1) \;+\; \sum_{i=1}^{b-1}\zeta_{\mathcal{A}}(a,i)\zeta_{\mathcal{A}}(b-i,c-1) \quad \text{(by Proposition 3)}\Big)\\
=\;& (-1)^{a-1}\sum_{j=1}^{k-2}\binom{j-1}{b-1}\binom{k-1-j}{a+b-j}Z_{\mathcal{A}}(j,k-1-j) \qquad (67)\\
&+ (-1)^{b-1}\sum_{j=2}^{k-3}\binom{j-1}{a}\binom{k-1-j}{a+b-j}Z_{\mathcal{A}}(j)\,Z_{\mathcal{A}}(k-1-j)
\end{aligned}$$

for $k=a+b+c$ odd. To obtain the regularized value of $\mathbb{B}(a,b,c-1)Z_{\mathcal{A}}(1)$, one needs a finite analogue of $\zeta'(a,s-a)\mid_{s=k}$. The same heuristic as before goes as

$$\begin{aligned}
\zeta'_{\leq}(a,k-a) &= \sum_{0<m\leq n} m^{-a}n^{-k+a}(-\log n) \text{ ``}\equiv\text{'' } \sum_{0<m\leq n} m^{p-1-a}n^{-k+a}(-\log n)\\
&\equiv \sum_{0<n}\Bigg(\sum_{i=1}^{k-a-1} b(p-1-i,a)\,n^{i-k+a}(-\log n) + \sum_{l=a-1}^{p-1-k+a} b(l,a)\,n^{p-1-l-k+a}(-\log n)\Bigg)\\
&\text{``}=\text{''} \sum_{i=1}^{k-a-1} b(p-1-i,a)\zeta'(k-a-i) + \sum_{l=a-1}^{p-1-k+a} b(l,a)\zeta'(-p+1+l+k-a)\,.
\end{aligned}$$

From this and by $b(p-1-i,a)=(-1)^a\binom{a+i}{a}Z_{\mathcal{A}}(a+i)$, we may set

$$\begin{aligned}
Z'_{\mathcal{A}}(a,k-a) &= Z'_{\mathcal{A},\leq}(a,k-a) \text{ ``}=\text{'' } \sum_{i=1}^{k-a-1}(-1)^a\binom{a+i}{a}Z_{\mathcal{A}}(a+i)\,Z'_{\mathcal{A}}(k-a-i)\\
&\qquad - \sum_{l=0}^{p-k}\Bigg(\frac{1}{a+l}\binom{a+l}{a}B_l\,\frac{(-1)^l}{p}\left(\frac{B_{p-k-l+1}}{p-k-l+1}-\frac{B_{2p-k-l}}{2p-k-l}\right)\Bigg)\,.
\end{aligned}$$

We still have the divergent term $(-1)^a\binom{k-1}{a}Z_{\mathcal{A}}(k-1)Z'_{\mathcal{A}}(1)$ in the first sum. To obtain the regularized value of this, we may need $Z''_{\mathcal{A}}(k-1)$ as well as the "Stieltjes constant $\gamma^{(1)}_{\mathcal{A}}$ in $\mathcal{A}$" defined in Example 8 in §1.

First, by using as before $\binom{s-1}{a}'=\binom{s-1}{a}(\psi(s)-\psi(s-a))$ and $\psi(s)-\psi(s-1)=\frac{1}{s-1}$, we compute

$$\begin{aligned}
\binom{k-\epsilon-1}{a} &= \binom{k-1}{a}\Bigg(1-(H_{k-1}-H_{k-a-1})\epsilon\\
&\qquad + \frac{1}{2}\big((H_{k-1}-H_{k-a-1})^2-(H^{(2)}_{k-1}-H^{(2)}_{k-a-1})\big)\epsilon^2 + O(\epsilon^3)\Bigg)\,,
\end{aligned}$$

where $H^{(2)}_m = 1+\frac{1}{2^2}+\cdots+\frac{1}{m^2}$. Hence, the regularized $\binom{k-1}{a}Z_{\mathcal{A}}(k-1)Z'_{\mathcal{A}}(1)$ should be

$$\begin{aligned}
&\binom{k-1}{a}\Bigg(-\frac{1}{2}\big((H_{k-1}-H_{k-a-1})^2-(H^{(2)}_{k-1}-H^{(2)}_{k-a-1})\big)Z_{\mathcal{A}}(k-1)\\
&\quad -(H_{k-1}-H_{k-a-1})Z'_{\mathcal{A}}(k-1)-\frac{1}{2}Z''_{\mathcal{A}}(k-1)-\gamma^{(1)}_{\mathcal{A}}Z_{\mathcal{A}}(k-1)\Bigg)\,.
\end{aligned}$$

The final form of $Z_{\mathcal{A}}(a,b,c)$ when $k=a+b+c$ is odd is:

$$\begin{aligned}
&Z_{\mathcal{A}}(a,b,c)\\
&\ = \widetilde{\mathbb{B}}(a,b,c) \;-\; Z_{\mathcal{A}}(a+b,c) \;-\; Z_{\mathcal{A}}(a,b+c) \;-\; Z_{\mathcal{A}}(k)\\
&\ -\sum_{i=1}^{b-1}\zeta_{\mathcal{A}}(a,i)\big(Z_{\mathcal{A}}(b-i,c) \;+\; Z_{\mathcal{A}}(b+c-i)\big) \;-\; \sum_{i=1}^{c-2}\mathbb{B}(a,b,i)\,Z_{\mathcal{A}}(c-i)\\
&\ +(-1)^a\sum_{j=1}^{k-2}\binom{j-1}{b-1}\binom{k-1-j}{c-1}\big((\gamma_{\mathcal{A}}-H_{k-1-j}+H_{c-1})Z_{\mathcal{A}}(j,k-1-j)-Z'_{\mathcal{A}}(j,k-1-j)\big)\\
&\ +(-1)^b\sum_{j=2}^{k-3}\binom{j-1}{a}\binom{k-1-j}{c-1}Z_{\mathcal{A}}(j)\big((\gamma_{\mathcal{A}}-H_{k-1-j}+H_{c-1})Z_{\mathcal{A}}(k-1-j)-Z'_{\mathcal{A}}(k-1-j)\big)\,.
\end{aligned}$$

6. The ring of $\mathcal{A}$-multiple zeta values: structural theorems

Structural theorems. For each integer $k\geq 0$, let $\mathfrak{Z}_{\mathcal{A},k}$ be the $\mathbb{Q}$-vector subspace of $\mathcal{A}$ spanned by the $\mathcal{A}$MZVs of weight k:

$$\mathfrak{Z}_{\mathcal{A},k}:=\sum_{r=0}^{k}\sum_{\substack{k_1,\dots,k_r\geq 1\\ k_1+\cdots+k_r=k}}\mathbb{Q}\,\zeta_{\mathcal{A}}(k_1,\dots,k_r)\,,$$

and set $\mathfrak{Z}_{\mathcal{A}}=\sum_{k\geq 0}\mathfrak{Z}_{\mathcal{A},k}$. Here we set $\zeta_{\mathcal{A}}(\emptyset)=1$, so $\mathfrak{Z}_{\mathcal{A},0}=\mathbb{Q}$.

Proposition 4. *For any indices* $\mathbf{k}$ *and* $\mathbf{l}$*, we have the series shuffle multiplication*

$$\zeta_{\mathcal{A}}(\mathbf{k})\zeta_{\mathcal{A}}(\mathbf{l}) \;=\; \zeta_{\mathcal{A}}(\mathbf{k}*\mathbf{l}). \tag{68}$$

In particular, the space $\mathfrak{Z}_{\mathcal{A}}$ *is a* $\mathbb{Q}$*-subalgebra of* $\mathcal{A}$*.*

Proof. This follows from the fact that the product of p-components (3) of two $\zeta_{\mathcal{A}}(\mathbf{k})$ and $\zeta_{\mathcal{A}}(\mathbf{l})$ is equal to the p-component of $\zeta_{\mathcal{A}}(\mathbf{k}*\mathbf{l})$, an example being $\zeta_p(a)\zeta_p(b)=\zeta_p(a,b)+\zeta_p(b,a)+\zeta_p(a+b)$. □

We note that exactly the same argument applies to $\mathcal{A}$MZVs with negative indices and the formula (68) is always true. But the conclusion that the a priori larger space of $\mathcal{A}$MZVs is also closed under multiplication is not so interesting because it is the same space, as we then show in Proposition 5.

Proposition 5. *For any index set* $(k_1,\dots,k_r)$ *with each* $k_i\in\mathbb{Z}$*, we have* $\zeta_{\mathcal{A}}(k_1,\dots,k_r)\in\mathfrak{Z}_{\mathcal{A}}$*.*

Proof. When all k_i are positive, the assertion is obvious by definition. We proceed by induction on the length of the index in general. If the length is 1, $\zeta_{\mathcal{A}}(k)$ is simply zero except $\zeta_{\mathcal{A}}(0)=-1$ and the proposition is true in both cases. When the length is larger than 1 and the ith index k_i is non-positive, we can sum up the partial sum $\sum_{m_{i-1}<m_i<m_{i+1}}m_i^{|k_i|}$ by using the Seki-Bernoulli formula and write it as a difference of polynomials in m_{i+1} and in m_{i-1}, which gives us lower depth sums. □

We remark that, if k_i's are not all positive, the expression of $\zeta_{\mathcal{A}}(k_1,\dots,k_r)$ as a linear combination of positive-indexed ones has mixed weights in general, a typical example being

$$\zeta_{\mathcal{A}}(3,-2,-3,6) \;=\; \frac{1}{6}\zeta_{\mathcal{A}}(1,6)-\frac{7}{8}\zeta_{\mathcal{A}}(1,4)-\frac{1}{8}\zeta_{\mathcal{A}}(1,2).$$

The next result is an analogue of the "parity theorem" for classical MZVs proved in [48] and [17]. Before giving it we formulate a lemma that will be used several times. Its formulation uses the "non-strict" or "Euler" version of $\mathcal{A}$MZV, which will be denoted by

$$\zeta^{\star}_{\mathcal{A}}(k_1,\dots,k_r) \;=\; \Bigl(\sum_{0<n_1\le\cdots\le n_r<p}\frac{1}{n_1^{k_1}\cdots n_r^{k_r}} \bmod p\Bigr)_{(p)}.$$

Lemma 2. *Let $(k_1,\dots,k_r)\in\mathbb{N}^r$ be any index of length r.*

1) We have

$$\sum_{i=0}^{r}\zeta_{\mathcal{A}}(k_1,\dots,k_i)\cdot(-1)^{r-i}\zeta^{\star}_{\mathcal{A}}(k_r,\dots,k_{i+1}) \;=\; 0. \tag{69}$$

2) Modulo the space of $\mathcal{A}$MZVs of length less than r, we have

$$\sum_{i=0}^{r}\zeta_{\mathcal{A}}(k_1,\dots,k_i)\cdot(-1)^{r-i}\zeta_{\mathcal{A}}(k_r,\dots,k_{i+1})\equiv 0.$$

Proof. The first identity comes from the definition and a property of the antipode in the abstract stuffle Hopf algebra ([14, Theorem 3.1]). As for the second, we note that the series shuffle multiplication (68) modulo lower length is simply the naive shuffle of indices, hence the claim reduces to the identity in [17, Lemma 2] in the group ring of the symmetric group. Alternatively, we can deduce 2) from 1) because $\zeta^{\star}_{\mathcal{A}}(k_r,\dots,k_{i+1})$ is congruent to $\zeta_{\mathcal{A}}(k_r,\dots,k_{i+1})$ modulo lower length $\mathcal{A}$MZVs. □

Proposition 6. *When the weight $k=k_1+\cdots+k_r$ and the length r have the same parity, the $\mathcal{A}$MZV $\zeta_{\mathcal{A}}(k_1,\dots,k_r)$ is a linear combination of $\mathcal{A}$MZVs having shorter length and products of $\mathcal{A}$MZVs the sum of whose weights is k and the sum of whose lengths is at most r.*

Proof. From 2) of the lemma, we have, modulo lower length and products of lower weights (note that $\zeta_{\mathcal{A}}(k)=0$ and so terms for $1\le i\le r-1$ are products of $\mathcal{A}$MZVs of weight and length less than $k-2$ and $r-2$ respectively),

$$\zeta_{\mathcal{A}}(k_1,\dots,k_r)+(-1)^r\zeta_{\mathcal{A}}(k_r,\dots,k_1) \;\equiv\; 0.$$

From this and the symmetry $\zeta_{\mathcal{A}}(k_r,\dots,k_1)=(-1)^k\zeta_{\mathcal{A}}(k_1,\dots,k_r)$ we obtain our assertion. □

Remark 1. According to the corollary of Theorem 4 in §7 **d** and our main conjecture (5), we expect a stronger parity statement that the $\mathcal{A}$MZV $\zeta_{\mathcal{A}}(k_1,\dots,k_r)$ of weight k and length r with $k\equiv r \pmod 2$ is a linear combination of $\mathcal{A}$MZVs having shorter length. However we cannot prove this yet.[6]

To illustrate, consider $\zeta_{\mathcal{A}}(a,b,c)$ with $a+b+c$ odd. Since any $\zeta_{\mathcal{A}}(k)$ vanishes, the identity (69) becomes $-\zeta^{\star}_{\mathcal{A}}(c,b,a)+\zeta_{\mathcal{A}}(a,b,c)=0$. But the symmetry $\zeta^{\star}_{\mathcal{A}}(c,b,a)=-\zeta^{\star}_{\mathcal{A}}(a,b,c)$ and the definition of $\zeta^{\star}_{\mathcal{A}}$ give $2\zeta_{\mathcal{A}}(a,b,c)+\zeta_{\mathcal{A}}(a+b,c)+\zeta_{\mathcal{A}}(a,b+c)=0$, which is Corollary 5 of Proposition 3.

[6]For length 4, Risan proved the stronger parity statement by heavily using computer algebra in his master's thesis (2025, Nagoya University, unpublished).

For usual MZVs there is a shuffle product ш such that $\zeta(\mathbf{k}ш\mathbf{l})=\zeta(\mathbf{k})\zeta(\mathbf{l})$ in the convergent case. (Warning: ш is not the usual shuffle! See §7 **a** for details.) We do not yet know any ш-product rule parallel to (68), but have the following shuffle relations. We conjecture that these relations together with (68) give all relations (algebraic or linear) among $\mathcal{A}$MZVs.

Theorem 2. *For any index sets* $\mathbf{k}$ *and* $\mathbf{l}$*, we have*

$$\zeta_{\mathcal{A}}(\mathbf{k}ш\mathbf{l}) \;=\; (-1)^{|\mathbf{l}|}\zeta_{\mathcal{A}}(\mathbf{k},\bar{\mathbf{l}}), \tag{70}$$

where $|\mathbf{l}|$ *is the weight of* $\mathbf{l}$ *and* $\bar{\mathbf{l}}$ *is the reversal of* $\mathbf{l}$*.*

Proof. We use the multiple polylogarithm series

$$\mathrm{Li}_{\mathbf{k}}(z) \;=\; \sum_{0<m_1<\cdots<m_r} \frac{z^{m_r}}{m_1^{k_1}\cdots m_r^{k_r}} \qquad (\mathbf{k}=(k_1,\dots,k_r))$$

and the facts that the p-component of $\zeta_{\mathcal{A}}(\mathbf{k})$ is equal to the sum modulo p of the coefficient of z^m in $\mathrm{Li}_{\mathbf{k}}(z)$ for $0<m<p$ and that the series $\mathrm{Li}_{\mathbf{k}}(z)$ satisfies the shuffle product rule: $\mathrm{Li}_{\mathbf{k}}(z)\mathrm{Li}_{\mathbf{l}}(z)=\mathrm{Li}_{\mathbf{k}ш\mathbf{l}}(z)$. Hence, setting $\mathbf{k}=(k_1,\dots,k_r)$ and $\mathbf{l}=(l_1,\dots,l_s)$ and working modulo p, we have

$$\begin{aligned}
\big(\zeta_{\mathcal{A}}(\mathbf{k}ш\mathbf{l})\big)_{(p)} \;&=\; \sum_{0<m<p}\big(\text{coefficient of } z^m \text{ in } \mathrm{Li}_{\mathbf{k}}(z)\mathrm{Li}_{\mathbf{l}}(z)\big)\\
&= \sum_{0<i,j,i+j<p}\Bigg(\sum_{0<m_1<\cdots<m_{r-1}<i}\frac{1}{m_1^{k_1}\cdots m_{r-1}^{k_{r-1}}i^{k_r}}\Bigg)\Bigg(\sum_{0<n_1<\cdots<n_{s-1}<j}\frac{1}{n_1^{l_1}\cdots n_{s-1}^{l_{s-1}}j^{l_s}}\Bigg)\\
&\equiv \sum_{0<i<j<p}\Bigg(\sum_{0<m_1<\cdots<m_{r-1}<i}\frac{1}{m_1^{k_1}\cdots m_{r-1}^{k_{r-1}}i^{k_r}}\Bigg)\Bigg(\sum_{j<n_{s-1}<\cdots<n_1<p}\frac{(-1)^{l_1+\cdots+l_s}}{j^{l_s}n_{s-1}^{l_{s-1}}\cdots n_1^{l_1}}\Bigg)\\
&= \sum_{0<m_1<\cdots<m_{r-1}<i<j<n_{s-1}<\cdots<n_1<p}\frac{(-1)^{l_1+\cdots+l_s}}{m_1^{k_1}\cdots m_{r-1}^{k_{r-1}}i^{k_r}j^{l_s}n_{s-1}^{l_{s-1}}\cdots n_1^{l_1}}\\
&= \big((-1)^{|\mathbf{l}|}\zeta_{\mathcal{A}}(\mathbf{k},\bar{\mathbf{l}})\big)_{(p)},
\end{aligned}$$

where the third line is obtained from the second by replacing j by $p-j$ and every n_i by $p-n_i$. □

We end this section by stating three conjectures about the relations satisfied by $\mathcal{A}$MZVs.

Conjecture 3. *All algebraic and linear relations among* $\mathcal{A}$*MZVs over* $\mathbb{Q}$ *can be deduced from* (68) *and* (70)*.*

Note that the relation (68) becomes ($\mathbb{Q}$-) linear if we restrict $\mathbf{l}$ to be of length 1 because then $\zeta_{\mathcal{A}}(\mathbf{l})=0$.

Conjecture 4. *All linear relations among* $\mathcal{A}$*MZVs over* $\mathbb{Q}$ *can be deduced from* (70) *and*

$$\zeta_{\mathcal{A}}(\mathbf{k}*(\ell)) \;=\; 0 \qquad \textit{for all } \ell\ge 1. \tag{71}$$

Conjecture 5. *It is even enough to use* (70) *and* (71) *for* ℓ *odd.*

In fact, in the computation done so far, it always suffice to use only (70) and (71) for $\ell=1$ and $\ell=3$, but this is probably just "the law of small numbers," since up to weight 11 it was even enough to use only $\ell=1$, but this fails in weight 12.

Part II: Finite real multiple zeta values

As explained in the introduction, the word "finite" before "multiple zeta value" has two different interpretations and the main theme of the paper is that there is a mysterious correspondence between them. In Part I we studied the first one, based on the analogues of multiple zeta values in finite fields. Now we turn to the second, based on the symmetrized zeta values (4), which are finite even though the individual summands may not. To study them, one needs the different notions of regularized multiple zeta values based on different product structures (naive shuffle, stuffle, and shuffle products) on formal multiple zeta sums. This material, most of which is well known, is reviewed in §7, and the symmetric multiple zeta values themselves are studied in the following section. In the remaining two sections we discuss some conjectural or provable properties of these finite real multiple zeta values and in particular their expected connections with their $\mathcal{A}$-analogues. A recurring theme here is the shift of depth as given in the statement of the main conjecture in the Introduction and also discussed in points **b.** and **g.** of §3.

7. Shuffle multiplications and regularization

There are two essentially different ways of multiplying classical MZVs that are called the shuffle and stuffle products and whose equality, with divergent cases being suitably taken into account, conjecturally gives all linear relations among MZVs. These were first noticed by Ecalle and the second author and their properties were further explored by them and several authors ([7], [31], [10], [39], [17], [11]).

a. Three shuffle multiplications

We first begin by recalling the "shuffle" and "stuffle" multiplications of multiple zeta values and the "extended double shuffle relations," which conjecturally suffice to describe all linear dependences of multiple zeta values over $\mathbb{Q}$. We will work with the $\mathbb{Q}$-vector space

$$\mathcal{R} \;=\; \bigoplus_{r\geq 0} \mathcal{R}^{(r)} \;=\; \bigoplus_{r\geq 0} \mathbb{Q}[\mathbb{N}^r]$$

of finite $\mathbb{Q}$-linear combinations of symbols $[\mathbf{k}] = [k_1, \ldots, k_r]$ with $\mathbf{k} = (k_1, \ldots, k_r) \in \mathbb{N}^r$ for some r. This space can be—and frequently is—identified either with the $\mathbb{Q}$-vector space $\langle z_1, z_2, \ldots \rangle_{\mathbb{Q}}$ of polynomials with integer coefficients in infinitely many non-commuting variables $z_1, z_2, \ldots$, by sending $[\mathbf{k}] = (k_1, \ldots, k_r)$ to $z_{k_1} \cdots z_{k_r}$, or alternatively with the $\mathbb{Q}$-vector space $y\langle x, y\rangle_{\mathbb{Q}}$ of polynomials with integer coefficients in two non-commuting variables x and y spanned by words beginning with y, by sending $[\mathbf{k}]$ to $yx^{k_1-1} \cdots yx^{k_r-1}$, but in this paper we will not make any use of non-commuting variables.

We will consider three commutative multiplications on $\mathcal{R}$. The first, which we will call the *naive shuffle product*, is the bilinear map $ш : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$ obtained by defining $[\mathbf{k}']ш[\mathbf{k}'']$ for $\mathbf{k}' = (k'_1, \ldots, k'_r)$ and $\mathbf{k}' = (k''_1, \ldots, k''_s)$ to be the sum of all symbols $[\mathbf{k}] = [k_1, \ldots, k_n]$ with $n = r + s$ obtained by dividing the set $\{1, \ldots, n\}$ into disjoint subsets R and S of cardinality r and s and putting the entries of $\mathbf{k}'$ and $\mathbf{k}''$ without changing their order into the positions labelled by R and S, respectively, a simple example being

$$[2,3]\,ш\,[5] \;=\; [2,3,5] \,+\, [2,5,3] \,+\, [5,2,3]\,.$$

With respect to this product, $\mathcal{R}$ becomes a commutative bigraded ring (graded by the weight and depth, where $[k_1, \ldots, k_r]$ has weight $k_1 + \cdots + k_r$ and depth r).

The second multiplication $*: \mathcal{R}\times\mathcal{R}\to\mathcal{R}$, called the *stuffle product*[7] or the *harmonic product*, sends $([\mathbf{k}'],[\mathbf{k}''])$ to the sum of $[\mathbf{k}']\text{Ш}[\mathbf{k}'']$ and lower depth terms obtained by allowing the sets R and S in the above description to overlap and adding the corresponding indices, a simple example being

$$[2,3]*[5] \;=\; \underbrace{[2,3,5]\;+\;[2,5,3]\;+\;[5,2,3]}_{[2,3]\,\text{Ш}\,[5]}+[7,3]\;+\;[2,8]\,.$$

With respect to this product, $\mathcal{R}$ becomes a commutative graded and filtered ring (graded by the weight and filtered by the depth), the difference being due to the fact that now the product of elements of depth r and s is no longer depth-homogeneous but is a sum of terms of depth $\le r+s$. It is clear from the definitions that the $\mathcal{A}$-evaluation map $\zeta_{\mathcal{A}}:\mathcal{R}\to\mathfrak{Z}_{\mathcal{A}}$ sending $[\emptyset]$ to 1 and $[\mathbf{k}]$ to $\zeta_{\mathcal{A}}(\mathbf{k})$ is a ring homomorphism with respect to this product. The same is true (and, of course, even more familiar) for the real-valued map sending $[\mathbf{k}]$ to the usual multiple zeta value $\zeta(\mathbf{k})$, except that now we must restrict the map to the $\mathbb{Z}$-submodule $\mathcal{R}_0$ of $\mathcal{R}$ spanned by the *admissible* symbols, i.e., by $[\emptyset]$ and the symbols $[k_1,\dots,k_r]$ with $k_r\ge 2$, in order that the sum defining $\zeta(\mathbf{k})$ be convergent. We will see in the next subsection how to extend the map $\zeta^{\mathbb{R}}:\mathcal{R}_0\to\mathbb{R}$ to an algebra homomorphism from the full $\mathcal{R}$ to $\mathbb{R}[T]$.

As we just said, the evaluation map $\zeta^{\mathbb{R}}:\mathcal{R}_0\to\mathfrak{Z}\subset\mathbb{R}$ is a ring homomorphism, i.e., we have $\zeta(\mathbf{k}'*\mathbf{k}'')=\zeta(\mathbf{k}')\zeta(\mathbf{k}'')$ for any two admissible indices $\mathbf{k}'$ and $\mathbf{k}''$. The same is not true for the multiplication Ш on $\mathcal{R}$ or $\mathcal{R}_0$, but it is true for a third product, the *shuffle product* ш, which we now define. The definition of ш and the proof of the identity $\zeta(\mathbf{k}'\,ш\,\mathbf{k}'')=\zeta(\mathbf{k}')\zeta(\mathbf{k}'')$ for convergent MZVs is based on their relation to the Drinfel'd integral discussed in **b** below, but there is also well-known purely algebraic definition that makes sense for any tuples of natural numbers; Transform any such tuple $\mathbf{k}=(k_1,\dots,k_r)$ into a sequence of 0s and 1s starting with 1 by replacing each k_i by a 1 followed by k_i-1 0s, and then multiply the $(0,1)$-sequences by the naive shuffle and transform back. The subring $\mathcal{R}_0$ corresponds to $(0,1)$-sequences starting with 1 and ending with 0, and is a subring of $\mathcal{R}$ with respect to the shuffle product ш. (Details can be found in many places, e.g.,[14,52].) The third interpretation of ш is based on the *multiple polylogarithm*

$$\mathrm{Li}_{\mathbf{k}}(z)\;=\;\sum_{0<m_1<\cdots<m_r}\frac{z^{m_r}}{m_1^{k_1}\cdots m_r^{k_r}}\quad(\mathbf{k}=(k_1,\dots,k_r))\,, \tag{72}$$

(which make sense as formal power series for both the rings $\mathcal{A}$ and $\mathbb{R}$), together with the identity

$$\mathrm{Li}_{\mathbf{k}}(z)\,\mathrm{Li}_{\mathbf{l}}(z)\;=\;\mathrm{Li}_{\mathbf{k}\text{Ш}\mathbf{l}}(z)\,. \tag{73}$$

This identity holds for any index sets $\mathbf{k}$ and $\mathbf{l}$, admissible or not, in the sense of formal power series but if both are admissible the series converges absolutely at $z=1$, and since $\mathrm{Li}_{\mathbf{k}}(1)=\zeta(\mathbf{k})$ we immediately deduce the desired product identity

$$\zeta(\mathbf{k})\,\zeta(\mathbf{l})\;=\;\zeta(\mathbf{k}\,ш\,\mathbf{l})\qquad(\mathbf{k},\,\mathbf{l}\in\mathcal{R}_0). \tag{74}$$

b. Integral representations of real MZVs

The usual definition of ш is based on the identity

$$\zeta(\mathbf{k})\;=\;\zeta(k_1,\dots,k_r)\;=\;I(\underbrace{1,0,\dots,0}_{k_1},\;\dots,\;\underbrace{1,0,\dots,0}_{k_r})\,, \tag{75}$$

[7] a term coined by David Broadhurst because thse are "sh**uffle** products with some extra **stuff**"

where $I(\varepsilon_1,\dots,\varepsilon_k)$ for $\varepsilon_a,\dots,\varepsilon_k\in\{0,1\}$ with $\varepsilon_1=1$ and $\varepsilon_k=0$ is the *Drinfel'd integral*

$$I(\varepsilon_1,\dots,\varepsilon_k) \;=\; \int_{0<t_1<\dots<t_k<1}\!\!\cdots\!\int \omega_1(t_1)\wedge\dots\wedge\omega_k(t_k) \qquad \Big(\omega_0(t)=\frac{dt}{t}\,,\quad \omega_1(t)=\frac{dt}{1-t}\Big)\,. \tag{76}$$

Multiplying two such integrals simply shuffles thier arguments ε_i. (There is no "stuffle" issue here since the sets of points where some arguments of the two integrands coincide has measure 0 and does not contribute to the integral.) This proves (74). If we are in the divergent case (where the last ε_k is no longer required to be 0), then we should interpret all of the zeta values as their shuffle-regularized values as explained in the next subsection. See also [17].

There is another way to define ⧢ using a different integral expression of $\zeta(\mathbf{k})$. To obtain it, we start from (75), write $x_1,\dots,x_r$ for the variables t_i in (76) for which $\varepsilon_i=1$, and carry out the integrations over the remaining variables t_i by using the identity

$$\int_{X<t_1<\dots<t_h<Y}\!\!\cdots\!\int \frac{dt_1}{t_1}\cdots\frac{dt_h}{t_h} \;=\; \frac{(\log Y/X)^h}{h!} \qquad (h\ge 0),$$

obtaining the less well-known alternative integral representation

$$\zeta(k_1,\dots,k_r) \;=\; \int_{0<x_1<\dots<x_r<x_{r+1}=1}\!\!\cdots\!\int \;\prod_{i=1}^{r}\Big(\frac{\log(x_{i+1}/x_i)^{k_i-1}}{(k_i-1)!}\;\frac{dx_i}{1-x_i}\Big) \tag{77}$$

which has the advantage over (75) of being r- rather than k-dimensional, where r is the depth of $\mathbf{k}$ and k its weight. Now consider the generating series

$$F_r(X_1,\dots,X_r) \;:=\; \sum_{k_1,\dots,k_r\ge 1}\zeta(k_1,\dots,k_r)\,X_1^{k_1-1}\cdots X_r^{k_r-1} \tag{78}$$

and $G_r(Y_1,\dots,Y_r) \;:=\; F_r(Y_1,Y_1+Y_2,\dots,Y_1+\dots+Y_r)$. Then (77) gives

$$G_r(Y_1,\dots,Y_r) \;=\; \int_{0<x_1<\dots<x_r<x_{r+1}=1}\!\!\cdots\!\int \frac{x_1^{-Y_1}}{1-x_1}\cdot\frac{x_2^{-Y_2}}{1-x_2}\cdots\frac{x_r^{-Y_r}}{1-x_r}\,dx_1\cdots dx_r. \tag{79}$$

Strictly speaking, equation (78) does not make sence since it includes the divergent integrals with $k_r=1$, so we should replace $\zeta(k_1,\dots,k_r)$ by $\mathrm{Li}_{\mathbf{k}}(e^{-\epsilon})$ in (78) and the upper limit of integration in (79) by $e^{-\epsilon}$, and iterpret all of the zeta values as their second regularization as explained below. (See [17] for more details.) From this integral representation, it is clear that the relation

$$G_r(Y_1,\dots,Y_r)G_r(Z_1,\dots,Z_s) \;=\; G_{r+s}((Y_1,\dots,Y_r)\,\text{Ш}\,(Z_1,\dots,Z_s)) \tag{80}$$

holds, where Ш is the naive shuffle. Then the alternative way to define ⧢ is as follows. Let

$$\Phi_r(X_1,\dots,X_r) \;:=\; \sum_{k_1,\dots,k_r\ge 1}[k_1,\dots,k_r]\,X_1^{k_1-1}\cdots X_r^{k_r-1} \;\in\; \mathcal{R}[X_1,\dots,X_r]$$

be the formal generating power series of indices of length r, and define a $\mathbb{Q}$-linear map ϕ from $\mathcal{R}$ to itself by (the collection of)

$$\Phi_r(X_1,X_1+X_2,\dots,X_1+\dots+X_r) \;=\; \sum_{k_1,\dots,k_r\ge 1}\phi([k_1,\dots,k_r])\,X_1^{k_1-1}\cdots X_r^{k_r-1},$$

the first values being

$$\phi([k]) = [k], \qquad \phi([k_1,k_2]) = \sum_{i=0}^{k_1-1} \binom{k_2+i-1}{i} [k_1-i, k_2+i],$$

$$\phi([k_1,k_2,k_3]) = \sum_{i=0}^{k_1+k_2-2} \sum_{j=0}^{k_1-1} \binom{k_3-1+i}{i} \binom{k_2-1+j}{j} [k_1-j, k_2-i+j, k_3+i].$$

Then the shuffle product $\mathbf{k}ш\mathbf{l}$ is equal to

$$\mathbf{k}ш\mathbf{l} \;=\; \phi^{-1}\big(\phi(\mathbf{k})Ш\phi(\mathbf{l})\big),$$

or, since ϕ is an isomorphism, we can *define* the bilinear product ш by this formula.

c. Regularized MZVs and the extended double shuffle relations

We recall briefly the two notions of regularized MZVs as discussed, in particular, in [17]. For every index set $\mathbf{k}$ there are two polynomials with real coefficients $\zeta^*(\mathbf{k};T)$ and $\zeta^{Ш}(\mathbf{k};T)$. These can be defined either axiomatically by the properties

- For $\mathbf{k}$ admissible both are constant polynomials (independent of T) and agree with $\zeta(\mathbf{k})$.
- both take on the value T if $\mathbf{k}=(1)$ (i.e., formally we are writing all divergent multiple zeta values as polynomials in $\zeta(1)$),
- they multiply according to the stuffle and shuffle rules, respectively,

or explicitly by the asymptotic formulas

$$\sum_{0<m_1<\cdots<m_r<M} \frac{1}{m_1^{k_1}\cdots m_r^{k_r}} \;=\; \zeta^*(\mathbf{k};\log M+\gamma) \,+\, \mathrm{o}(1) \qquad \text{as } M\to\infty \tag{81}$$

and

$$\mathrm{Li}_{\mathbf{k}}(1-\epsilon) \;=\; \sum_{0<m_1<\cdots<m_r} \frac{(1-\epsilon)^{m_r}}{m_1^{k_1}\cdots m_r^{k_r}} \;=\; \zeta^{Ш}(\mathbf{k};\log(1/\epsilon)) \,+\, \mathrm{o}(1) \quad \text{as } \epsilon\to 0\,, \tag{82}$$

where γ is Euler's constant. These polynomials have the further properties:

(i) For $\mathbf{k} = (\mathbf{k}', \underbrace{1,\ldots,1}_{s})$ with $\mathbf{k}'$ admissible and $s\ge 0$, $\zeta^*(\mathbf{k};T)$ and $\zeta^{Ш}(\mathbf{k};T)$ both have degree s with leading term $\zeta(\mathbf{k}')T^s/s!$.

(ii) For both $\bullet = *$ and ш, we have the identity of generating functions

$$\sum_{s=0}^{\infty} \zeta^{\bullet}(\mathbf{k},\underbrace{1,\ldots,1}_{s};T)\,x^s \;=\; e^{Tx}\sum_{s=0}^{\infty} \zeta^{\bullet}(\mathbf{k},\underbrace{1,\ldots,1}_{s})\,x^s, \tag{83}$$

where we define the regularized value $\zeta^{\bullet}(\mathbf{k}) \in \mathfrak{Z}$ to be $\zeta^{\bullet}(\mathbf{k};0)$.

(iii) The two normalizations are related by $\zeta^{Ш}(\mathbf{k};T) = \rho(\zeta^*(\mathbf{k};T))$, where $\rho : \mathbb{R}[T]\to\mathbb{R}[T]$ is the $\mathbb{R}$-linear map defined by

$$\rho\big(e^{Tu}\big) \;=\; A(u)\,e^{Tu}\,, \tag{84}$$

where $A(u)$ is the power series in $\mathbb{R}[[u]]$ defined by

$$\begin{aligned} A(u) \;&=\; e^{\gamma u}\,\Gamma(1+u) \;=\; \exp\bigg(\sum_{n=2}^{\infty} \frac{(-1)^n}{n}\,\zeta(n)\,u^n\bigg) \\ &=\; 1 \,+\, \frac{\pi^2}{12}\,u^2 \,-\, \frac{\zeta(3)}{3}\,u^3 \,+\, \frac{\pi^4}{160}\,u^4 \,-\, \bigg(\frac{\pi^2\zeta(3)}{36}+\frac{\zeta(5)}{5}\bigg)\,u^5 \,+\, \cdots\,. \end{aligned} \tag{85}$$

Explicitly, (84) says that ρ sends T^n to $\sum_{m=0}^{n}\binom{n}{m}\alpha_m T^{n-m}$, where $A(u) = \sum_{m=0}^{\infty}\alpha_m \frac{u^m}{m!}$. In terms of the generating function in (ii), this can be written as

$$\sum_{i=0}^{\infty}\zeta^{ш}(\mathbf{k},\underbrace{1,\dots,1}_{i})x^i \;=\; A(x)\sum_{i=0}^{\infty}\zeta^{*}(\mathbf{k},\underbrace{1,\dots,1}_{i})x^i. \tag{86}$$

(iv) Each coefficient of the polynomials $\zeta^*(\mathbf{k};T)$ and $\zeta^{ш}(\mathbf{k};T)$ is an integral linear combination of multiple zeta values $\zeta(\mathbf{k}')$ with $\mathbf{k}'$ admissible, and there is an explicit algebraic algorithm to determine these coefficients.

d. Depth and parity

Recall that the depth of a multiple zeta value is usually defined as the length of its argument (but sometimes defined as r if the value is the product of $\zeta(2)^n$ times a multiple zeta value of length r) and that it is subadditive but not additive, meaning that the ring of real multiple zeta values is filtered but not graded by the depth. An important fact is the "depth-parity relationship", which says that the minimal depth of a multiple zeta value (meaning the minimum of the maximum depth of the terms of any expression for it as a sum of other multiple zeta values) always has the same parity of the weight. The weaker statement modulo products was proved by Tsumura [48] and in [17] and can be found in many places, and the full statement was proved in even more generality (for multiple polylogarithms rather than just multiple zeta values) by Erik Panzer [37, Theorem 1.1], but for completeness and it is very short, we include the proof of the strengthening here.

Proposition 7. *If $\mathbf{k}$ has weight k and depth $r \not\equiv k \pmod 2$ then $\zeta(\mathbf{k})$ has depth $\le r-1$ mod π^2.*

Proof. We proceed by induction on the weight. The case $k = 2$ is trivial. Suppose the statement holds for weight smaller than k. By the parity result just cited, we know that the depth of $\zeta(\mathbf{k})$ modulo products is $\le r-1$ if $k \not\equiv r \pmod 2$, and these products $\zeta(\mathbf{k}')\zeta(\mathbf{k}'')$ have weight and depth (k', r') and (k'', r'') with $k' + k'' = k$ and $r' + r'' \le r$. If $r' + r'' = r$, then either $k' \not\equiv r \pmod 2$ or $k'' \not\equiv r'' \pmod 2$ holds because k and r have opposite parity. And then the corresponding factor $\zeta(\mathbf{k}')$ or $\zeta(\mathbf{k}'')$ is congruent modulo π^2 to something of lower depth by the induction hypothesis, and we are done. $\square$

We note that Panzer [37, Eq. (1.12)] gives a complete reduction formula in the case of depth 3. However, his formula, reduced modulo π^2, looks more complicated than our conjectural formula in Conjecture 2 in §5.

8. Symmetric multiple zeta values

Definition. *For any index $(k_1,\dots,k_r) \in \mathbb{N}^r$, we define the $\bullet$-symmetric multiple zeta value by*

$$S^\bullet(k_1,\dots,k_r) \;=\; \sum_{i=0}^{r}(-1)^{k_{i+1}+\cdots+k_r}\zeta^\bullet(k_1,\dots,k_i;T)\,\zeta^\bullet(k_r,\dots,k_{i+1};T)\,, \tag{87}$$

where $\bullet = *$ or ш.

The symmetry $S^\bullet(k_1,\dots,k_r) = (-1)^{k_1+\cdots+k_r}S^\bullet(k_r,\dots,k_1)$ is obvious from the definition (hence the name). These are *a priori* elements in $\mathfrak{Z}[T] \subset \mathbb{R}[T]$, but the following theorem says that they are in fact independent of T, justifying the notation.

Theorem 3. *The sums defined by the right-hand side of* (87) *belong to* $\mathfrak{Z}$ *for both* $\bullet = *$ *and* ш, *and their values agree modulo the ideal generated by* $\pi^2 = 6\zeta(2)$.

Proof. If there are no 1's in the index, this is clear and both values agree. Suppose $\mathbf{k}$ is of the form $\mathbf{k} = (\mathbf{l}, \underbrace{1,\ldots,1}_{j}, \overline{\mathbf{m}})$ with $\mathbf{l}$ and $\mathbf{m}$ admissible and $j \geq 1$, where $\overline{\mathbf{m}}$ is the reversal of $\mathbf{m}$. We see that the partial sum

$$\sum_{i=0}^{j} \zeta^{\bullet}(\mathbf{l}, \underbrace{1,\ldots,1}_{i}; T) \cdot (-1)^{|\mathbf{m}|+j-i} \zeta^{\bullet}(\mathbf{m}, \underbrace{1,\ldots,1}_{j-i}; T) \quad (|\mathbf{m}| = \text{the weight of } \mathbf{m})$$

is already finite, because this sum is equal to the coefficient of x^j in

$$\begin{aligned}
&(-1)^{|\mathbf{m}|} \sum_{i_1=0}^{\infty} \zeta^{\bullet}(\mathbf{l}, \underbrace{1,\ldots,1}_{i_1}; T) x^{i_1} \cdot \sum_{i_2=0}^{\infty} \zeta^{\bullet}(\mathbf{m}, \underbrace{1,\ldots,1}_{i_2}; T) (-x)^{i_2} \\
&= (-1)^{|\mathbf{m}|} e^{Tx} \sum_{i_1=0}^{\infty} \zeta^{\bullet}(\mathbf{l}, \underbrace{1,\ldots,1}_{i_1}) x^{i_1} \cdot e^{-Tx} \sum_{i_2=0}^{\infty} \zeta^{\bullet}(\mathbf{m}, \underbrace{1,\ldots,1}_{i_2}) (-x)^{i_2} \\
&= (-1)^{|\mathbf{m}|} \sum_{i_1=0}^{\infty} \zeta^{\bullet}(\mathbf{l}, \underbrace{1,\ldots,1}_{i_1}) x^{i_1} \cdot \sum_{i_2=0}^{\infty} \zeta^{\bullet}(\mathbf{m}, \underbrace{1,\ldots,1}_{i_2}) (-x)^{i_2},
\end{aligned}$$

which is visibly independent of T. For the first equality, we have used the identity (83) in §7.

The second assertion can be obtained from (86) in §7, which gives

$$\begin{aligned}
&\sum_{i_1=0}^{\infty} \zeta^{ш}(\mathbf{l}, \underbrace{1,\ldots,1}_{i_1}) x^{i_1} \cdot \sum_{i_2=0}^{\infty} \zeta^{ш}(\mathbf{m}, \underbrace{1,\ldots,1}_{i_2}) (-x)^{i_2} \\
&= \Gamma(1+x)\Gamma(1-x) \sum_{i_1=0}^{\infty} \zeta^{*}(\mathbf{l}, \underbrace{1,\ldots,1}_{i_1}) x^{i_1} \cdot \sum_{i_2=0}^{\infty} \zeta^{*}(\mathbf{m}, \underbrace{1,\ldots,1}_{i_2}) (-x)^{i_2}.
\end{aligned}$$

Since the coefficients of the Taylor series of $\Gamma(1+x)\Gamma(1-x) = \pi x/\sin \pi x$ are in the ideal (π^2), we obtain the theorem. □

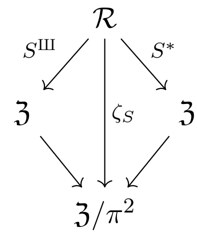
Corollary. *If there are no consecutive* 1*'s in the index* $\mathbf{k}$*, the two values* $S^*(\mathbf{k})$ *and* $S^{ш}(\mathbf{k})$ *coincide.*

Proof. This follows from the formulas in the above proof and the fact that the Taylor series of $\Gamma(1+x)\Gamma(1-x)$ contains only even powers of x. □

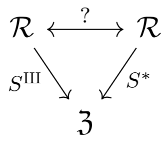
Set $\mathfrak{Z}^{\mathrm{red}} = \mathfrak{Z}/(\pi^2)$. Then Theorem 3 implies that we can define a map $\zeta_S : \mathcal{R} \to \mathfrak{Z}^{\mathrm{red}}$ by

$$\zeta_S(\mathbf{k}) \;=\; \big(S^*(\mathbf{k}) \text{ or } S^{ш}(\mathbf{k}) \mod \pi^2\big) \quad \in \quad \mathfrak{Z}^{\mathrm{red}}\,. \tag{88}$$

We call $\zeta_S(\mathbf{k})$ the *symmetric multiple zeta value* or the *finite real multiple zeta value.*



Remark 2. One might ask if there are regularization maps from $\mathcal{R}$ to $\mathcal{R}$ in one or both directions under which S^* and $S^{ш}$ correspond in such a way that the following diagram commutes.



Example 2. For $k \geq 1$, the depth 1 value $S^\bullet(k)$ for either $\bullet = ш$ or $\bullet = *$ is computed as

$$S^\bullet(k) \;=\; (-1)^k \zeta^\bullet(k;T) + \zeta^\bullet(k;T) \;=\; \begin{cases} 0 & \text{if } k \text{ is odd,} \\ 2\zeta(k) & \text{if } k \text{ is even.} \end{cases}$$

Since $\zeta(k) \in \pi^2\mathfrak{Z}$ for even k by Euler, we have $\zeta_S(k) = 0$.

For depth 2, we compute $S^*(a, b)$ as

$$S^*(a,b) \;=\; (-1)^{a+b}\zeta^*(b,a;T) + (-1)^b\zeta^*(a;T)\zeta^*(b;T) + \zeta^*(a,b;T).$$

First suppose $a + b$ is even. If both a and b are even (and hence greater than 1), then the right-hand side is equal to

$$\zeta(b,a) + \zeta(a)\zeta(b) + \zeta(a,b) \;=\; 2\zeta(a)\zeta(b) - \zeta(a+b),$$

which is congruent to $0 \mod \pi^2$. If both a and b are odd, then $S^*(a, b)$ is equal to

$$\zeta^*(b,a;T) - \zeta^*(a;T)\zeta^*(b;T) + \zeta^*(a,b;T) \;=\; -\zeta(a+b),$$

which is again $0 \mod \pi^2$. Suppose $a + b$ is odd. Then either a or b is even and so $S^*(a, b)$ is congruent modulo π^2 to $\zeta^*(a, b; T) - \zeta^*(b, a; T)$. When both a and b are greater than 1, we see from [51, Proposition 7] that

$$\zeta(a,b) - \zeta(b,a) \;\equiv\; (-1)^b\binom{a+b}{a}\zeta(a+b) \pmod{\pi^2}.$$

Computation (which we omit) using the regularized polynomial shows that the same formula holds for $a = 1$ or $b = 1$, and from all these we conclude

$$\zeta_S(a,b) \;=\; (-1)^b\binom{a+b}{a}\zeta(a+b) \bmod \pi^2. \tag{89}$$

Theorem 4. *The depth of $\zeta_S(k_1, \dots, k_r) \in \mathfrak{Z}^{\mathrm{red}}$ is at most $r - 1$.*

Proof. By Proposition 7, we may replace the factor $(-1)^{k_{i+1}+\cdots+k_r}\zeta^\bullet(k_r, \dots, k_{i+1})$ in the definition of $S^\bullet(k_1, \dots, k_r)$ by $(-1)^{r-i}\zeta^\bullet(k_r, \dots, k_{i+1})$ when we work modulo lower depths and π^2 (note that the parity theorem holds true also for regularized values). Then, the conclusion follows from exactly the same argument as in the proof of Proposition 6 in §6. □

Corollary. *If the weight $k = k_1 + \cdots + k_r$ and the length r has the same parity, the symmetric multiple zeta value $\zeta_S(k_1, \ldots, k_r)$ has depth at most $r-2$. Moreover, $\zeta_S(k_1, \ldots, k_r)$ is a linear combination of $\zeta_S(\mathbf{l})$s with $\mathbf{l}$s of length at most $r-1$.*

Proof. The first statement follows from Proposition 7. The second follows from Yasuda's refinement (personal communication in 2016) of his theorem in [50], that for either $\bullet = ш$ or $*$, the $S^\bullet(k_1, \ldots, k_r)$s with fixed values of r and of $k = k_1 + \cdots + k_r$ generate the space of MZVs of weight k and depth $r-1$ modulo π^2. □

Proposition 8. *We have*

$$S^*(\mathbf{k})\,S^*(\mathbf{l}) \;=\; S^*(\mathbf{k} * \mathbf{l}) \tag{90}$$

for any two index sets $\mathbf{k}$ and $\mathbf{l}$, so that the maps $S^* : \mathcal{R} \to \mathfrak{Z}$ and $\zeta_S : \mathcal{R} \to \mathfrak{Z}^{\mathrm{red}}$ are algebra homomorphisms.

Proof. We can prove this purely algebraically, although rather tediously, by showing the map

$$[k_1, \ldots, k_r] \mapsto \sum_{i=0}^{r} (-1)^{k_{i+1}+\cdots+k_r}\,[k_1, \ldots, k_i] * [k_r, \ldots, k_{i+1}]$$

is a $*$-homomorphism from $\mathcal{R}_* = (\mathcal{R}, *)$ to itself by induction on the sum of lengths of indices. Or more conceptually, this is a consequence of the fact that the algebra $\mathcal{R}_*$ becomes a Hopf algebra with the deconcatenation coproduct

$$[k_1, \ldots, k_r] \mapsto \sum_{i=0}^{r} [k_1, \ldots, k_i] \otimes [k_{i+1}, \ldots, k_r]$$

(see [14, §3]) and that the map $[k_1, \ldots, k_j] \mapsto (-1)^{k_1 \cdots + k_j}[k_j, \ldots, k_1]$ is a $*$-homomorphism. Another transparent way is to look at the expression of $S^*(\mathbf{k})$ as the limit of the sum with a new ordering of non-zero integers, which we present as a proposition below. □

Proposition 9. *We have*

$$S^*(k_1, \ldots, k_r) \;=\; \lim_{N\to\infty} \sum_{\substack{m_1 \prec \cdots \prec m_r \\ 0<|m_i|<N}} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}}, \tag{91}$$

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

$$1 \prec 2 \prec 3 \prec \;\cdots\; \prec -3 \prec -2 \prec -1\,.$$

Proof.[8] For each positive integer N, we write $\zeta_N^{\pm}(k_1, \ldots, k_r)$ for the sum appearing on the right of (91), which by definition is equal to

$$\zeta_N^{\pm}(k_1, \ldots, k_r) \;=\; \sum_{i=0}^{r} (-1)^{k_{i+1}+\cdots+k_r} \zeta_N(k_1, \ldots, k_i)\,\zeta_N(k_r, \ldots, k_{i+1}).$$

Since we know from (81) that for each index $\mathbf{k}$ we have

$$\zeta_N(\mathbf{k}) \;=\; \zeta^*(\mathbf{k}; \log N + \gamma) + \mathrm{o}(1) \qquad \text{as } N \to \infty,$$

[8]The proof here is simpler than our original one. We thank Shuji Yamamoto for the suggestion.

we conclude that

$$\begin{aligned}&\zeta_N^{\pm}(k_1,\dots,k_r)\\&=\sum_{i=0}^{r}(-1)^{k_{i+1}+\cdots+k_r}\zeta^*(k_1,\dots,k_i;\log N+\gamma)\zeta^*(k_r,\dots,k_{i+1};\log N+\gamma)+\mathrm{o}(1)\end{aligned}$$

as $N\to\infty$. We already know from Theorem 3 that the sum on the right is independent of N and equals $S^*(k_1,\dots,k_r)$. Hence by taking the limit $N\to\infty$, we have

$$\lim_{N\to\infty}\zeta_N^{\pm}(k_1,\dots,k_r) \;=\; S^*(k_1,\dots,k_r)$$

as desired. □

Theorem 5. *For any index sets* $\mathbf{k}$ *and* $\mathbf{l}$*, we have*

$$S^{ш}(\mathbf{k}ш\mathbf{l}) \;=\; (-1)^{|\mathbf{l}|}S^{ш}(\mathbf{k},\bar{\mathbf{l}}), \tag{92}$$

where $|\mathbf{l}|$ *and* $\bar{\mathbf{l}}$ *denote the weight and the reversal of* $\mathbf{l}$ *respectively.*

Proof. For each i with $0\le i\le r$, define a linear map $S_i^{(r)}:\mathcal{R}^{(r)}\to\mathcal{R}^{(r)}$ by

$$S_i^{(r)}([k_1,\dots,k_r]) \;=\; (-1)^{k_{i+1}+\cdots+k_r}\,[k_1,\dots,k_i]ш[k_r,\dots,k_{i+1}],$$

and set $S^{(r)}=\sum_{i=0}^{r}S_i^{(r)}$ so that

$$S^{(r)}([k_1,\dots,k_r]) \;=\; \sum_{i=0}^{r}(-1)^{k_{i+1}+\cdots+k_r}\,[k_1,\dots,k_i]ш[k_r,\dots,k_{i+1}].$$

Since the shuffle regularization map $\zeta^{ш}:\mathcal{R}\to\mathbb{R}[T]$ defined by $\mathbf{k}\mapsto\zeta^{ш}(\mathbf{k};T)$ satisfies the ш-product rule $\zeta^{ш}(\mathbf{k}ш\mathbf{l};T)=\zeta^{ш}(\mathbf{k};T)\zeta^{ш}(\mathbf{l};T)$ (see §7 **c**), we have $S^{ш}(\mathbf{k})=\zeta^{ш}(S^{(r)}(\mathbf{k}))$ if $\mathbf{k}$ has depth r and the identity (92) in the theorem is equivalent (by replacing $\mathbf{l}$ by $(-1)^{|\mathbf{l}|}\bar{\mathbf{l}}$ and setting $\mathbf{k}=[k_1,\dots,k_i]$ and $\mathbf{l}=[k_{i+1},\dots,k_r]$) to the identity of maps $\zeta^{ш}\circ S^{(r)}\circ S_i^{(r)}=\zeta^{ш}\circ S^{(r)}$ for any i. In the following, we show the stronger statement that the identity $S^{(r)}\circ S_i^{(r)}=S^{(r)}$ is already true at the level of maps of formal algebra $\mathcal{R}$, by reducing this to a classical identity in the group algebra of the symmetric group.

Proposition 10. *For* $r\ge 1$ *and* $0\le i\le r$*, we have the identity of linear maps*

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

on $\mathcal{R}^{(r)}$*.*

Proof. Consider the generating function of indices of length r

$$F(x_1,\dots,x_r) \;=\; \sum_{k_1,\dots,k_r\ge 1}[k_1,\dots,k_r]\,x_1^{k_1-1}\cdots x_r^{k_r-1}\;\in\;\mathcal{R}[x_1,\dots,x_r].$$

We use the same notations $S_i^{(r)}$ and $S^{(r)}$ for the coefficient-wise extension of these maps to power series, and show the identity $S^{(r)}\big(S_i^{(r)}F\big)=S^{(r)}F$ for each i with $0\le i\le r$. For this, we introduce new variables y_i such that $x_i=y_1+\cdots+y_i$ and set

$$G(y_1,\dots,y_r) \;=\; F(y_1,y_1+y_2,\dots,y_1+\cdots+y_r).$$

Then, the shuffle product is encoded as the identity

$$G(y_1,\dots,y_i)\,G(y_{i+1},\dots,y_r) \;=\; \big(G\,|_{sh_i^{(r)}}\big)(y_1,\dots,y_r) \tag{93}$$

in $\mathcal{R}_{ш}[y_1,\dots,y_r]$ (this is a formal version of (80)), where the coefficient ring is the space of indices $\mathcal{R}$ endowed with the commutative shuffle product ш. Here, $sh_i^{(r)}$ is an element in the group algebra $\mathbb{Z}[\mathfrak{S}_r]$ of the symmetric group $\mathfrak{S}_r$ (thought of as the permutation group of $\{1,\dots,r\}$) defined by $sh_i^{(r)} = \sum_{\sigma\in Sh_i^{(r)}}\sigma$, where $Sh_i^{(r)}$ is the set of "$(i,r-i)$-shuffles"

$$Sh_i^{(r)} \;=\; \{\sigma\in\mathfrak{S}_r \mid \sigma(1)<\cdots<\sigma(i),\,\sigma(i+1)<\cdots<\sigma(r)\}.$$

The action of the group algebra $\mathbb{Z}[\mathfrak{S}_r]$ on the power series ring is the right action $(f|_\sigma)(y_1,\dots,y_r) = f(y_{\sigma^{-1}(1)},\dots,y_{\sigma^{-1}(r)})$, extended linearly.

Now we introduce a new variable y_{r+1} satisfying $y_1+\cdots+y_r+y_{r+1}=0$, and consider the action of $\mathfrak{S}_{r+1}$. Specifically, apply the element $\rho_i^{(r)} = (1,\dots,i,r+1,\dots,i+1)\in\mathfrak{S}_{r+1}$ on both sides of (93). Then the left-hand side becomes

$$\begin{aligned}
&G(y_1,\dots,y_i)\,G(y_{r+1},y_r,\dots,y_{i+2})\\
&= F(y_1,y_1+y_2,\dots,y_1+\cdots+y_i)\,F(y_{r+1},y_{r+1}+y_r,\dots,y_{r+1}+\cdots+y_{i+2})\\
&= F(x_1,x_2,\dots,x_i)\,F(-x_r,-x_{r-1},\dots,-x_{i+1})\\
&= (-1)^{r-i}S_i^{(r)}F(x_1,\dots,x_r).
\end{aligned}$$

On the other hand, the right-hand side will be equal to $(G|_{u_i^{(r)}})(y_1,\dots,y_r)$, where $u_i^{(r)} = sh_i^{(r)}\circ\rho_i^{(r)} = \sum_{\sigma\in\mathcal{U}_i^{(r)}}\sigma$ and $\mathcal{U}_i^{(r)} = Sh_i^{(r)}\circ\rho_i^{(r)}$ is the set of 'unimodal' elements in $\mathfrak{S}_{r+1}$ given by

$$\mathcal{U}_i^{(r)} \;=\; \{\sigma\in\mathfrak{S}_{r+1} \mid \sigma(1)<\cdots<\sigma(i+1)>\cdots>\sigma(r+1)\}.$$

Here, we have identified $\mathfrak{S}_r$ with the subset of $\mathfrak{S}_{r+1}$ fixing $r+1$. We therefore have

$$S_i^{(r)}F = (G|_{(-1)^{r-i}u_i^{(r)}})(y_1,\dots,y_r), \tag{94}$$

and by summing over i

$$S^{(r)}F \;=\; (G|_{u_{\mathrm{alt}}^{(r)}})(y_1,\dots,y_r), \tag{95}$$

where $u_{\mathrm{alt}} = \sum_{i=0}^r(-1)^{r-i}u_i^{(r)}$. Applying the linear map $S^{(r)}$ on both sides of (94) and using (95) on the right (note that the linear action of $S^{(r)}$ commutes with changes and permutations of variables), we obtain $S^{(r)}\big(S_i^{(r)}F\big) = (G|_{u_{\mathrm{alt}}^{(r)}\circ(-1)^{r-i}u_i^{(r)}})(y_1,\dots,y_r)$. From a classical result essentially due to Specht (see [40, Lemma 8.18]), we have $u_{\mathrm{alt}}^{(r)}\circ(-1)^{r-i}u_i^{(r)} = u_{\mathrm{alt}}^{(r)}$, and hence the identity $S^{(r)}\big(S_i^{(r)}F\big) = S^{(r)}F$ is proved. □

This concludes the proof of Theorem 5. □

Observe that (90) and (92) are identical in form to (68) and (70) in §6, which is at the root of the conjectural isomorphism (12). We will discuss this in more depth in the next section.

Because of the conjectural identification of the two rings $\mathfrak{Z}_{\mathcal{A}}$ and $\mathfrak{Z}^{\mathrm{red}}$, any proven or conjectural identities in the former ring is expected to hold in the latter one as well. In particular, this should be true for each of the identities among $\mathcal{A}$MZVs discussed in §3. Without going too much into the details, we summarize the current state of knowledge for each of the identities in **b** to **e** of §3.

b: That $\zeta_{\mathcal{A}}(k)=0$ for all $k\geq 1$ and the formula (48) for $\zeta_{\mathcal{A}}(a,b)$ correspond to the identities in Example 2 under the correspondence $Z_{\mathcal{A}}(k)\leftrightarrow\zeta(k) \bmod \pi^2$. The next case, the relation

$$2\,\zeta_S(a,b,c) \;=\; -\,\zeta_S(a,b+c)\;-\;\zeta_S(a+b,c) \qquad \text{for } a+b+c \text{ odd},$$

which corresponds to (49), is also easily proved by direct computation of $S^*(a,b,c)$, using the "antipode relation" (the identity (69) for ζ^*).

c: The ζ_S-versions of equation (50) was proved by Murahara [32] and of equation (51) by Fujita-Komori [12].

d: As already mentioned, the symmetry (52) for ζ_S is obvious from the definition. The ζ_S-counterpart of the duality (53) was proved by Jarossay [19]. A ζ_S-analogue of Ohno's relation was proved by Oyama [36].

e: As far as the authors know, there seem to have been no attempt to establish identities like (55) in the ζ_S-setting.

As perhaps the strongest evidence for our Main Conjecture, we mention the work of Bachmann-Takeyama-Tasaka [4], where they introduced a *single* object (q-series) which specializes both to $\mathcal{A}$MZV and symmetric MZV.

9. Conjectural isomorphisms

Let $\mathcal{R}_*$ be the $\mathbb{Q}$-algebra of the space of indices equipped with the stuffle product $*$. In the following, we discuss conjectural structures of the $\mathbb{Q}$-algebras $\mathfrak{Z}_{\mathcal{A}}$ and $\mathfrak{Z}^{\mathrm{red}}$.

Consider the $\mathbb{Q}$-linear map $\zeta_{\mathcal{A}}:\mathcal{R}_*\ni\mathbf{k}\mapsto\zeta_{\mathcal{A}}(\mathbf{k})\in\mathfrak{Z}_{\mathcal{A}}$ which is an algebra homomorphism, and let $\mathfrak{I}^{\mathcal{A}}$ be the kernel of $\zeta_{\mathcal{A}}$. Let J be the $\mathbb{Q}$-vector subspace of $\mathcal{R}_*$ spanned by the elements $\mathbf{k}\,⧢\,\mathbf{l}-(-1)^{|\mathbf{l}|}[\mathbf{k},\bar{\mathbf{l}}]$:

$$J \;:=\; \Big\langle \mathbf{k}\,⧢\,\mathbf{l}-(-1)^{|\mathbf{l}|}[\mathbf{k},\bar{\mathbf{l}}]\;|\;\mathbf{k},\mathbf{l}\in\mathcal{R}\Big\rangle_{\mathbb{Q}},$$

and $\mathfrak{I}$ be the $*$-ideal of $\mathcal{R}_*$ generated by J. We know by (70) that J, and hence $\mathfrak{I}$, is contained in $\mathfrak{I}^{\mathcal{A}}$. We conjecture that $\mathfrak{I}$ is the exact kernel.

Conjecture 6. *We have $\mathfrak{I}^{\mathcal{A}}=\mathfrak{I}$ and hence an isomorphism of $\mathbb{Q}$-algebras*

$$\mathcal{R}_*/\mathfrak{I}\;\simeq\;\mathfrak{Z}_{\mathcal{A}}.$$

In §6, we conjectured in Cojecture 4 that the kernel $\mathfrak{I}^{\mathcal{A}}$ is spanned by J and all $\mathbf{k}*[l]$ ($\forall\mathbf{k}$ and $l\geq 1$). The following shows the latter elements are indeed contained in $\mathfrak{I}$.

Proposition 11. *The ideal $\mathfrak{I}$ contains $[l]$ for all $l\in\mathbb{N}$.*

Proof. When $\mathbf{k}=\emptyset$ and $\mathbf{l}=[1]$, the element $\mathbf{k}\,⧢\,\mathbf{l}-(-1)^{|\mathbf{l}|}[\mathbf{k},\bar{\mathbf{l}}]$ becomes $2[1]$, thus $[1]$ is contained in $J\subset\mathfrak{I}$ (the same argument shows $[l]\in J$ for any odd l). We proceed by induction. Take $\mathbf{k}=[l-1]$ and $\mathbf{l}=[1]$ to get

$$\mathbf{k}\,⧢\,\mathbf{l}-(-1)^{|\mathbf{l}|}[\mathbf{k},\bar{\mathbf{l}}] \;=\; 2[l-1,1]+[l-2,2]+\cdots+[2,l-2]+2[1,l-1]\in J.$$

On the other hand, for $1\leq i\leq l-1$, we have by induction hypothesis and the stuffle product that

$$[l-i]*[i] \;=\; [l-i,i]+[i,l-i]+[l]\in\mathfrak{I}.$$

These two together imply $[l]\in\mathfrak{I}$. $\square$

We remark that J and $\mathfrak{J}$ are different already at weight 2. The element [2] is contained in $\mathfrak{J}$ but not in J. Consider the following intermediate subspaces J_1, J_2, J_3 between J and $\mathfrak{J}$:

$$\begin{aligned} J_1 &= J + \langle \mathbf{k} * [1] \mid \mathbf{k} \in \mathcal{R} \rangle_{\mathbb{Q}}\,, \\ J_2 &= J + \langle \mathbf{k} * [l] \mid \mathbf{k} \in \mathcal{R},\ l \text{ odd} \rangle_{\mathbb{Q}}\,, \\ J_3 &= J + \langle \mathbf{k} * [l] \mid \mathbf{k} \in \mathcal{R},\ l \in \mathbb{N} \rangle_{\mathbb{Q}}\,, \end{aligned}$$

so that $J \subset J_1 \subseteq J_2 \subseteq J_3 \subseteq \mathfrak{J}$. The conjectures at the end of §6 say that the last two of these inclusions are in fact equalities.

Next consider the case of $\mathfrak{Z}^{\mathrm{red}} = \mathfrak{Z}/(\pi^2)$. Let s^* and $s^{ш}$ be the two $\mathbb{Q}$-linear maps from $\mathcal{R}$ to $\mathcal{R}_0$ given by

$$s^{\bullet}([k_1,\dots,k_r]) \;=\; \sum_{i=0}^{r} (-1)^{k_{i+1}+\cdots+k_r} [k_1,\dots,k_i] \bullet [k_r,\dots,k_{i+1}] \qquad (\bullet = * \text{ or } ш),$$

of which s^* is a $*$-homomorphism (see the proof of Proposition 8). The maps S^* and $S^{ш}$ in §8 are therefore $S^* = \zeta \circ s^*$ and $S^{ш} = \zeta \circ s^{ш}$. Proposition 10 shows that $J \subseteq \ker(s^{ш})$. The next proposition says that this is in fact an equality:

Proposition 12. *The kernel of $s^{ш}$ is equal to J.*

Proof. Proposition 10 says that the map $\frac{1}{r+1}s^{ш}$ on the space $\mathcal{R}^{(r)}$ of depth r indices is an idempotent. Thus $\ker(s^{ш}) \cap \mathcal{R}^{(r)} = (\mathrm{Id} - \frac{1}{r+1}s^{ш})(\mathcal{R}^{(r)})$. Since $J^{(r)}$, the depth r subspace of J, is spanned by $(S_i^{(r)} - \mathrm{Id})(\mathbf{k})$ for $0 \le i \le r$ and $\mathbf{k} \in \mathcal{R}^{(r)}$, the proposition follows. $\square$

Let $\overline{\zeta} : \mathcal{R}_0 \to \mathfrak{Z}^{\mathrm{red}}$ be the composition of the evaluation $\mathcal{R}_0 \ni \mathbf{k} \mapsto \zeta(\mathbf{k}) \in \mathfrak{Z}$ and the natural projection $\mathfrak{Z} \to \mathfrak{Z}^{\mathrm{red}} = \mathfrak{Z}/\pi^2\mathfrak{Z}$. We know by Theorem 3 that both $\overline{\zeta} \circ s^*$ and $\overline{\zeta} \circ s^{ш}$ give the same $\mathbb{Q}$-linear map ζ_S from $\mathcal{R}$ to $\mathfrak{Z}^{\mathrm{red}}$, which is an algebra homomorphism with respect to the $*$-product on $\mathcal{R}_*$. Let $\mathfrak{J}^S$ be the kernel of ζ_S.

Conjecture 7. *We have $\mathfrak{J}^S = \mathfrak{J}$, and hence an isomorphism of $\mathbb{Q}$-algebras*

$$\mathcal{R}_*/\mathfrak{J} \;\simeq\; \mathfrak{Z}^{\mathrm{red}}.$$

Here is a different conjectural description of the algebra $\mathfrak{Z}^{\mathrm{red}}$. Consider the restriction of $\overline{\zeta}$ to the subalgebra $s^*(\mathcal{R}) \subset \mathcal{R}_0$, and let $\mathfrak{J}_0^S$ be its kernel. We know by Theorem 3 and Theorem 5 that $(s^* - s^{ш})(\mathcal{R}) \cap s^*(\mathcal{R}), s^*(J)$, and $s^*(\mathfrak{J})$ are all contained in $\mathfrak{J}_0^S$. Our next conjecture is that all these coincide, in particular $s^*(J)$ is already a $*$-ideal of $s^*(\mathcal{R})$.

Conjecture 8. *We have $s^*(J) = s^*(\mathfrak{J}) = (s^* - s^{ш})(\mathcal{R}) \cap s^*(\mathcal{R})$, and an isomorphism of $\mathbb{Q}$-algebras*

$$s^*(\mathcal{R})/s^*(J) \;\simeq\; s^*(\mathcal{R})/\big((s^* - s^{ш})(\mathcal{R}) \cap s^*(\mathcal{R})\big) \;\simeq\; \mathfrak{Z}^{\mathrm{red}}\,.$$

Since $s^{ш}(J) = \{0\}$, we have an inclusion $s^*(J) \subset (s^* - s^{ш})(\mathcal{R}) \cap s^*(\mathcal{R})$ and also an obvious inclusion $s^*(J) \subset s^*(\mathfrak{J})$. We however do not know if $s^*(\mathfrak{J}) \subset (s^* - s^{ш})(\mathcal{R}) \cap s^*(\mathcal{R})$ holds, because we are not able to show that $(s^* - s^{ш})(\mathcal{R}) \cap s^*(\mathcal{R})$ is a $*$-ideal of $s^*(\mathcal{R})$.

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