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A Note on $\mathcal{F}_n$-multiple Zeta Values

by

Masataka ONO, Kosuke SAKURADA and Shin-ichiro SEKI

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Abstract. For several evaluations of special values and several relations known only in $\mathcal{A}_n$-multiple zeta values or $\mathcal{S}_n$-multiple zeta values, we prove that they are uniformly valid in $\mathcal{F}_n$-multiple zeta values for both the case where $\mathcal{F} = \mathcal{A}$ and $\mathcal{F} = \mathcal{S}$. In particular, the Bowman–Bradley type theorem and sum formulas for $\mathcal{S}_2$-multiple zeta values are proved.

1. Introduction

We call a tuple of positive integers $\boldsymbol{k} = (k_1, \dots, k_r)$ an *index*. We call $\mathrm{wt}(\boldsymbol{k}) := k_1 + \cdots + k_r$ (resp. $\mathrm{dep}(\boldsymbol{k}) := r$) the *weight* (resp. *depth*) of $\boldsymbol{k}$. If the condition $k_r \geq 2$ is satisfied, then we state that the index $\boldsymbol{k} = (k_1, \dots, k_r)$ is *admissible*. For an admissible index $\boldsymbol{k} = (k_1, \dots, k_r)$, the *multiple zeta value* (MZV) $\zeta(\boldsymbol{k})$ and the *multiple zeta-star value* (MZSV) $\zeta^\star(\boldsymbol{k})$ are defined by

$$\zeta(\boldsymbol{k}) := \sum_{0<n_1<\cdots<n_r} \frac{1}{n_1^{k_1} \cdots n_r^{k_r}}, \qquad \zeta^\star(\boldsymbol{k}) := \sum_{1\leq n_1\leq\cdots\leq n_r} \frac{1}{n_1^{k_1} \cdots n_r^{k_r}}.$$

These series are convergent. We set $\zeta(\varnothing) = \zeta^\star(\varnothing) = 1$ for the empty index $\varnothing$ (= the empty tuple).

First we recall the definition of $\mathcal{A}_n$*-multiple zeta(-star) values* ($\mathcal{A}_n$-MZ(S)Vs) introduced by Rosen; see [Ro, Se]. For a positive integer n, set

$$\mathcal{A}_n := \prod_p \mathbb{Z}/p^n\mathbb{Z} \Bigg/ \bigoplus_p \mathbb{Z}/p^n\mathbb{Z},$$

where p runs over all prime numbers. For an index $\boldsymbol{k} = (k_1, \dots, k_r)$, the $\mathcal{A}_n$-MZV $\zeta_{\mathcal{A}_n}(\boldsymbol{k})$ and the $\mathcal{A}_n$-MZSV $\zeta^\star_{\mathcal{A}_n}(\boldsymbol{k})$ are defined by

$$\zeta_{\mathcal{A}_n}(\boldsymbol{k}) := \left(\sum_{0<n_1<\cdots<n_r<p} \frac{1}{n_1^{k_1} \cdots n_r^{k_r}} \bmod p^n \right)_p,$$

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$$\zeta^{\star}_{\mathcal{A}_n}(\boldsymbol{k}) := \left(\sum_{1\le n_1\le\cdots\le n_r\le p-1} \frac{1}{n_1^{k_1}\cdots n_r^{k_r}} \bmod p^n \right)_p$$

as elements of $\mathcal{A}_n$. We also set $\zeta_{\mathcal{A}_n}(\varnothing) = \zeta^{\star}_{\mathcal{A}_n}(\varnothing) = 1$.

Next we recall the definition of *t-adic symmetric multiple zeta values* ($\widehat{\mathcal{S}}$-MZVs) introduced by Jarossay [J2]. Let t be an indeterminate. For $\bullet \in \{*, ш\}$ and an index $\boldsymbol{k} = (k_1, \dots, k_r)$, set

$$\zeta^{\bullet}_{\widehat{\mathcal{S}}}(\boldsymbol{k}) = \sum_{i=0}^{r} (-1)^{k_{i+1}+\cdots+k_r} \zeta^{\bullet}(k_1, \dots, k_i) \\ \times \sum_{l_{i+1},\dots,l_r\ge 0} \left[\prod_{j=i+1}^{r} \binom{k_j+l_j-1}{l_j} \right] \zeta^{\bullet}(k_r+l_r, \dots, k_{i+1}+l_{i+1}) t^{l_{i+1}+\cdots+l_r} \in \mathcal{Z}[\![t]\!].$$

Here, $\mathcal{Z}$ is the $\mathbb{Q}$-subalgebra of $\mathbb{R}$ generated by all MZVs and $\zeta^*(\boldsymbol{k}) \in \mathcal{Z}$ (resp. $\zeta^{ш}(\boldsymbol{k}) \in \mathcal{Z}$) is the harmonic (resp. shuffle) regularized MZV. See Subsection 2.1 for details. It is known that $\zeta^*_{\widehat{\mathcal{S}}}(\boldsymbol{k}) - \zeta^{ш}_{\widehat{\mathcal{S}}}(\boldsymbol{k}) \in (\zeta(2)\mathcal{Z})[\![t]\!]$ for any index $\boldsymbol{k}$ ([J2, Proposition 3.2.4] and [OSY, Proposition 2.1]). Thus,

$$\zeta_{\widehat{\mathcal{S}}}(\boldsymbol{k}) := \zeta^{\bullet}_{\widehat{\mathcal{S}}}(\boldsymbol{k}) \bmod \zeta(2)$$

is independent of the choice of the regularization $\bullet \in \{*, ш\}$ and defines a well-defined element of $\overline{\mathcal{Z}}[\![t]\!] := (\mathcal{Z}/\zeta(2)\mathcal{Z})[\![t]\!]$. We call $\zeta_{\widehat{\mathcal{S}}}(\boldsymbol{k})$ the $\widehat{\mathcal{S}}$-MZV. We also define the *t-adic symmetric multiple zeta-star value* ($\widehat{\mathcal{S}}$-MZSV) $\zeta^{\star}_{\widehat{\mathcal{S}}}(\boldsymbol{k})$ by

$$\zeta^{\star}_{\widehat{\mathcal{S}}}(k_1, \dots, k_r) = \sum_{\substack{\square \text{ is either a comma `,'} \\ \text{or a plus `+'}}} \zeta_{\widehat{\mathcal{S}}}(k_1 \square \cdots \square k_r).$$

See [HMO, Definition 1.1] for another equivalent definition of the $\widehat{\mathcal{S}}$-MZSV. For a positive integer n, let $\pi_n : \overline{\mathcal{Z}}[\![t]\!] \twoheadrightarrow \overline{\mathcal{Z}}[\![t]\!]/(t^n)$ be the natural projection.

DEFINITION 1.1. For an index $\boldsymbol{k} = (k_1, \dots, k_r)$, we define the *$\mathcal{S}_n$-multiple zeta(-star) value* ($\mathcal{S}_n$-MZ(S)V) by

$$\zeta_{\mathcal{S}_n}(\boldsymbol{k}) := \pi_n\big(\zeta_{\widehat{\mathcal{S}}}(\boldsymbol{k})\big), \quad \zeta^{\star}_{\mathcal{S}_n}(\boldsymbol{k}) := \pi_n\big(\zeta^{\star}_{\widehat{\mathcal{S}}}(\boldsymbol{k})\big) = \sum_{\substack{\square \text{ is either a comma `,'} \\ \text{or a plus `+'}}} \zeta_{\mathcal{S}_n}(k_1 \square \cdots \square k_r).$$

Note that $\zeta_{\mathcal{S}_1}(\boldsymbol{k})$ coincides with the usual symmetric multiple zeta value (SMZV) $\zeta_{\mathcal{S}}(\boldsymbol{k})$ defined by Kaneko and Zagier [KZ].

$\mathcal{A}_n$-MZ(S)Vs and $\mathcal{S}_n$-MZ(S)Vs are the main objects of this article and together they are called $\mathcal{F}_n$-MZ(S)Vs; $\mathcal{F}$ derives from the first letter of the word "finite". Similar to the conjecture [OSY, Conjecture 4.3], it is conjectured that $\mathcal{A}_n$-MZVs and $\mathcal{S}_n$-MZVs satisfy relations of the same form. Hence, a relation among $\mathcal{A}_n$-MZVs or $\mathcal{S}_n$-MZVs is always described collectively as a relation of $\mathcal{F}_n$-MZVs, at least conjecturally. The purpose of this paper is to confirm that several evaluations of special values and several relations known only in $\mathcal{A}_n$-MZVs or $\mathcal{S}_n$-MZVs are uniformly valid in $\mathcal{F}_n$-MZVs. In some cases, we only deal with $n = 1, 2, 3$.

The remainder of the paper is structured as follows. In Section 2, we prepare relevant tools including Zagier's formula for MZVs, the double shuffle relation for $\mathcal{F}_n$-MZVs and the relation for $\mathcal{F}_n$-MZVs derived from the antipode. In Section 3, we put forward some explicit evaluations of $\mathcal{F}_n$-MZ(S)Vs. In Section 4, we prove the Bowman–Bradley type theorem for $\mathcal{F}_2$-MZ(S)Vs. In Section 5, we prove sum formulas for $\mathcal{F}_n$-MZ(S)Vs with respect to specific n. Some complicated but elementary calculations for binomial coefficients (= the proof of Proposition A.1) are proved in the Appendix.

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2. Preliminaries

In this section, we prepare tools which are used in the following sections.

2.1. Algebraic setup

First we recall the notion of the harmonic algebra introduced in [H1]. Let $\mathfrak{H}^1 := \mathbb{Q} + e_1\mathbb{Q}\langle e_0, e_1\rangle \supset \mathfrak{H}^0 := \mathbb{Q}+e_1\mathbb{Q}\langle e_0, e_1\rangle e_0$, where $\mathbb{Q}\langle e_0, e_1\rangle$ is a non-commutative polynomial algebra in two variables e_0 and e_1. For a positive integer k, we set $e_k := e_1 e_0^{k-1}$. We define the harmonic product $*$ on $\mathfrak{H}^1$ by $w * 1 = 1 * w = w$, $e_{k_1}w_1 * e_{k_2}w_2 = e_{k_1}(w_1 * e_{k_2}w_2) + e_{k_2}(e_{k_1}w_1 * w_2) + e_{k_1+k_2}(w_1 * w_2)$ (w, w_1, w_2 are words in $\mathfrak{H}^1$, $k_1, k_2 \in \mathbb{Z}_{>0}$) with $\mathbb{Q}$-bilinearity. We also define the shuffle product $⧢$ on $\mathbb{Q}\langle e_0, e_1\rangle$ by $w ⧢ 1 = 1 ⧢ w = w$, $u_1w_1 ⧢ u_2w_2 = u_1(w_1 ⧢ u_2w_2) + u_2(u_1w_1 ⧢ w_2)$ (w, w_1, w_2 are words in $\mathbb{Q}\langle e_0, e_1\rangle$, $u_1, u_2 \in \{e_0, e_1\}$) with $\mathbb{Q}$-bilinearity. Let $\bullet \in \{*, ⧢\}$. It is known that $\mathfrak{H}^1$ becomes a commutative $\mathbb{Q}$-algebra with respect to the multiplication $\bullet$, which is denoted by $\mathfrak{H}^1_\bullet$. The subspace $\mathfrak{H}^0$ of $\mathfrak{H}^1$ is closed under $\bullet$ and becomes a $\mathbb{Q}$-subalgebra of $\mathfrak{H}^1_\bullet$, which is denoted by $\mathfrak{H}^0_\bullet$. We define Muneta's shuffle product $\widetilde{⧢}$ on $\mathfrak{H}^1$ ([Mun, §3]) by $w\widetilde{⧢}1 = 1\widetilde{⧢}w = w$, $e_{k_1}w_1\widetilde{⧢}e_{k_2}w_2 = e_{k_1}(w_1\widetilde{⧢}e_{k_2}w_2) + e_{k_2}(e_{k_1}w_1\widetilde{⧢}w_2)$ (w, w_1, w_2 are words in $\mathfrak{H}^1$, $k_1, k_2 \in \mathbb{Z}_{>0}$) with $\mathbb{Q}$-bilinearity.

Next, we recall the harmonic (resp. shuffle) regularized MZV introduced in [IKZ]. It is known that $\mathfrak{H}^1_\bullet \cong \mathfrak{H}^0_\bullet[e_1]$ as a $\mathbb{Q}$-algebra (see [H1] for $\bullet = *$ and [Re] for $\bullet = ⧢$). Therefore, for $\bullet \in \{*, ⧢\}$, any $a \in \mathfrak{H}^1_\bullet$ has a unique expression $a = \sum_{i=0}^n a_i \bullet e_1^{\bullet i}$, where $n \in \mathbb{Z}_{\geq 0}$, $a_i \in \mathfrak{H}^0_\bullet$ $(0 \leq i \leq n)$ and $e_1^{\bullet i} := \overbrace{e_1 \bullet \cdots \bullet e_1}^{i}$. By this expression, we define a $\mathbb{Q}$-algebra homomorphism $\mathrm{reg}_\bullet\colon \mathfrak{H}^1_\bullet \cong \mathfrak{H}^0_\bullet[e_1] \to \mathfrak{H}^0_\bullet$ by $\mathrm{reg}_\bullet\left(\sum_{i=0}^n a_i \bullet e_1^{\bullet i}\right) := a_0$. We set $e_{\boldsymbol{k}} := e_{k_1}\cdots e_{k_r}$ for a non-empty index $\boldsymbol{k} = (k_1, \ldots, k_r)$ and $e_\varnothing := 1$. Then we define a $\mathbb{Q}$-linear map $Z\colon \mathfrak{H}^0 \to \mathbb{R}$ by $Z(e_{\boldsymbol{k}}) := \zeta(\boldsymbol{k})$ for any admissible index $\boldsymbol{k}$. By using this terminology, we define the harmonic (resp. shuffle) regularized MZV $\zeta^*(\boldsymbol{k})$ (resp. $\zeta^⧢(\boldsymbol{k})$) by $\zeta^*(\boldsymbol{k}) = (Z \circ \mathrm{reg}_*)(e_{\boldsymbol{k}})$ (resp. $\zeta^⧢(\boldsymbol{k}) := (Z \circ \mathrm{reg}_⧢)(e_{\boldsymbol{k}})$) for any index $\boldsymbol{k}$.

To calculate the shuffle regularized MZV, we use the following fact.

LEMMA 2.1 (Regularization formula, [IKZ, Proposition 8]). *Let* $w = w'e_0$ *be an element of* $\mathfrak{H}^0$ *with* $w' \in \mathfrak{H}^1$. *Then, for a non-negative integer* m, *we have*

$$\mathrm{reg}_{ш}(we_1^m) = (-1)^m (w' ш e_1^m)e_0.$$

2.2. Zagier's formulas for MZVs

We quote some results on MZVs. We use these results to evaluate some $\mathcal{S}_1$-MZ(S)Vs and $\mathcal{S}_2$-MZ(S)Vs.

THEOREM 2.2 ([Z, Theorem 1]). *For non-negative integers* a *and* b, *we have*

$$\zeta(\{2\}^a, 3, \{2\}^b) = 2\sum_{r=1}^{a+b+1}(-1)^r\left\{\binom{2r}{2a+2} - \left(1-\frac{1}{2^{2r}}\right)\binom{2r}{2b+1}\right\}\zeta(\{2\}^{a+b-r+1})\zeta(2r+1),$$

where $\{2\}^a$ *denotes a repetitions* $\underbrace{2,\dots,2}_{a}$. *In particular, we have*

$$\begin{aligned}(2.1)\quad &\zeta(\{2\}^a, 3, \{2\}^b)\\ &\equiv 2(-1)^{a+b+1}\left\{\binom{2a+2b+2}{2a+2} - \left(1-\frac{1}{4^{a+b+1}}\right)\binom{2a+2b+2}{2b+1}\right\}\zeta(2a+2b+3) \bmod \zeta(2).\end{aligned}$$

THEOREM 2.3 ([Z, Proposition 7]). *Let* m *and* n *be positive integers with* $n \geq 2$ *and* $k := m+n$ *being odd. Define a positive integer* K *as* $k = 2K+1$. *Then we have*

$$\zeta(m,n) = (-1)^m \sum_{s=0}^{K-1}\left\{\binom{k-2s-1}{m-1} + \binom{k-2s-1}{n-1} - \delta_{n,2s} + (-1)^m\delta_{s,0}\right\}\zeta(2s)\zeta(k-2s).$$

Here $\delta_{x,y}$ *is Kronecker's delta, and we understand* $\zeta(0) = -\frac{1}{2}$. *In particular, we have*

$$\zeta(m,n) \equiv (-1)^{m+1}\frac{1}{2}\left\{\binom{k}{m} + (-1)^m\right\}\zeta(k) \bmod \zeta(2). \tag{2.2}$$

2.3. Double shuffle relation for $\mathcal{F}_n$-MZVs

The double shuffle relation (DSR) for $\mathcal{F}_n$-MZVs with $\mathcal{F} \in \{\mathcal{A}, \mathcal{S}\}$ established by Jarossay is a key tool in this paper. We define $\mathbb{Q}$-linear maps $Z_{\mathcal{A}_n} : \mathfrak{H}^1 \to \mathcal{A}_n$ and $Z_{\mathcal{S}_n} : \mathfrak{H}^1 \to \overline{\mathcal{Z}}[[t]]/(t^n)$ by

$$Z_{\mathcal{A}_n}(e_{\boldsymbol{k}}) := \zeta_{\mathcal{A}_n}(\boldsymbol{k}), \qquad Z_{\mathcal{S}_n}(e_{\boldsymbol{k}}) := \zeta_{\mathcal{S}_n}(\boldsymbol{k})$$

for any index $\boldsymbol{k}$.

THEOREM 2.4 (DSR for $\mathcal{F}_n$-MZVs, [J2]. cf. [OSY, Theorems 1.3 and 1.9]). *For indices* $\boldsymbol{k}$ *and* $\boldsymbol{l} = (l_1, \dots, l_s)$ *and a positive integer* n, *we have the harmonic relation for* $\mathcal{F}_n$-*MZVs*

$$Z_{\mathcal{F}_n}(e_{\boldsymbol{k}} * e_{\boldsymbol{l}}) = Z_{\mathcal{F}_n}(e_{\boldsymbol{k}})Z_{\mathcal{F}_n}(e_{\boldsymbol{l}}) \tag{2.3}$$

and the shuffle relation for $\mathcal{F}_n$-MZVs

$$Z_{\mathcal{F}_n}(e_{\boldsymbol{k}} \sqcup\!\sqcup\, e_{\boldsymbol{l}}) = (-1)^{\mathrm{wt}(\boldsymbol{l})} \sum_{\substack{\boldsymbol{l}'=(l'_1,\dots,l'_s)\in\mathbb{Z}^s_{\geq 0}\\ \mathrm{wt}(\boldsymbol{l}')\leq n-1}} \left[\prod_{j=1}^{s}\binom{l_j+l'_j-1}{l'_j}\right] Z_{\mathcal{F}_n}(e_{\boldsymbol{k}}e_{\overline{\boldsymbol{l}+\boldsymbol{l}'}})x_{\mathcal{F}_n}^{\mathrm{wt}(\boldsymbol{l}')}. \tag{2.4}$$

Here, we set $\mathrm{wt}(\boldsymbol{l}') \coloneqq l'_1+\cdots+l'_s$, $\overline{\boldsymbol{l}+\boldsymbol{l}'} \coloneqq (l_s+l'_s,\dots,l_1+l'_1)$ *and*

$$x_{\mathcal{F}_n} \coloneqq \begin{cases} \boldsymbol{p}_n \coloneqq (p \bmod p^n)_p & \text{if } \mathcal{F}=\mathcal{A},\\ t \bmod t^n & \text{if } \mathcal{F}=\mathcal{S}.\end{cases}$$

We refer to the case $\boldsymbol{k}=\varnothing$ of the shuffle relation as the *reversal formula*.

We also use the following relation for $\mathcal{F}_n$-MZVs.

PROPOSITION 2.5. *For an index $\boldsymbol{k}=(k_1,\dots,k_r)$, $n\in\mathbb{Z}_{\geq 1}$ and $\mathcal{F}\in\{\mathcal{A},\mathcal{S}\}$, we have*

$$\sum_{i=0}^{r}(-1)^i\zeta_{\mathcal{F}_n}(k_1,\dots,k_i)\zeta^{\star}_{\mathcal{F}_n}(k_r,\dots,k_{i+1})=0.$$

Proof. This follows from the harmonic relation and [IKOO, Proposition 6] (Note that the sign of [IKOO, Proposition 6] is mistaken). The case $\mathcal{F}=\mathcal{A}$ was first mentioned in [SS, Corollary 3.16 (42)]. □

3. Special values

In this section, we explicitly evaluate some $\mathcal{F}_n$-MZ(S)Vs. For positive integers n and k, set

$$\mathfrak{z}_{\mathcal{F}_n}(k) \coloneqq \begin{cases} \left(\dfrac{B_{p^{n-1}(p-1)-k+1}}{k-1+p^{n-1}} \bmod p^n\right)_p \in \mathcal{A}_n & \text{if } \mathcal{F}=\mathcal{A},\\ \zeta(k) \bmod \zeta(2) \in \overline{\mathcal{Z}}[[t]]/(t^n) & \text{if } \mathcal{F}=\mathcal{S}.\end{cases}$$

Here, B_j is the j-th Seki–Bernoulli number and $\widehat{B}_j$ denotes $\frac{B_j}{j}$.

PROPOSITION 3.1. *Let n and k be positive integers. For $1\leq l\leq n-1$,*

$$\mathfrak{z}_{\mathcal{A}_n}(k+l)\boldsymbol{p}_n^l = \sum_{j=1}^{n-l}(-1)^j\binom{n-l}{j}\left(\widehat{B}_{j(p-1)-k-l+1}\cdot p^l \bmod p^n\right)_p \in \mathcal{A}_n$$

holds. In particular,

$$\mathfrak{z}_{\mathcal{A}_2}(k+1)\boldsymbol{p}_2 = \left(\frac{B_{p-k-1}}{k+1}\cdot p \bmod p^2\right)_p \in \mathcal{A}_2.$$

Proof. Let p be a sufficiently large prime number. Then, by using the Kummer-type congruence proved by Zhi-Hong Sun [Su, Corollary 4.1], we have

$$\frac{B_{p^{n-1}(p-1)-k-l+1}}{k+l-1+p^{n-1}}\cdot p^l$$

$$\equiv (-1)^{n+l} \sum_{j=1}^{n-l} (-1)^{j-1} \binom{p^{n-1}-1-j}{n-l-j} \binom{p^{n-1}-1}{j-1} \widehat{B}_{j(p-1)-k-l+1} \cdot p^l \pmod{p^n}.$$

Since

$$(-1)^{n+l-1} \binom{p^{n-1}-1-j}{n-l-j} \binom{p^{n-1}-1}{j-1} \equiv \binom{n-l}{j} \pmod{p^{n-1}},$$

we have the desired formula. □

3.1. Depth 1 case

THEOREM 3.2. *For positive integers n and k, we have*

$$\zeta_{\mathcal{F}_n}(k) = (-1)^k \sum_{l=1}^{n-1} \binom{k+l-1}{l} \mathfrak{Z}_{\mathcal{F}_n}(k+l) x_{\mathcal{F}_n}^l.$$

Proof. The case $\mathcal{F} = \mathcal{A}$ is a special case of [W, Theorem 1]. Nevertheless, we can state the direct proof as follows. Let p be a sufficiently large prime number. By Euler's formula and Faulhaber's formula, we have

$$\begin{aligned} \sum_{m=1}^{p-1} \frac{1}{m^k} &\equiv \sum_{m=1}^{p-1} m^{\varphi(p^n)-k} \\ &\equiv \frac{1}{\varphi(p^n)-k+1} \sum_{l=1}^{n-1} \binom{\varphi(p^n)-k+1}{l} B_{\varphi(p^n)-k-l+1} \cdot p^l \\ &= -\sum_{l=1}^{n-1} \binom{\varphi(p^n)-k}{l} \frac{B_{\varphi(p^n)-k-l+1}}{k+l-1+p^{n-1}} \cdot p^l \pmod{p^n}, \end{aligned}$$

where φ is Euler's totient function. By a simple congruence

$$\binom{\varphi(p^n)-k}{l} \equiv (-1)^l \binom{k+l-1}{l} \pmod{p^{n-1}}$$

and the fact that B_j vanishes for odd $j \geq 3$, we have the desired equality in $\mathcal{A}_n$. Since the case $\mathcal{F} = \mathcal{S}$ is clear by definition, this completes the proof. □

REMARK 3.3. By combining the case $\mathcal{F} = \mathcal{A}$ of Theorem 3.2 and Proposition 3.1, we have

$$\sum_{m=1}^{p-1} \frac{1}{m^k} \equiv (-1)^k \sum_{l=1}^{n-1} \binom{k+l-1}{l} \sum_{j=1}^{n-l} (-1)^j \binom{n-l}{j} \widehat{B}_{j(p-1)-k-l+1} \cdot p^l \pmod{p^n}$$

for a sufficiently large prime p. We can check that this holds for $p \geq n+k+1$. This congruence is a generalization of [Su, Theorem 5.1 (a) and Remark 5.1] and [Tau, Theorem 2.1]. However, the proof is identical to that put forward by Sun.

3.2. Depth 2 case

Let $\tau_n : \overline{\mathcal{Z}}[[t]] \to \overline{\mathcal{Z}}[t]$ be the truncation map defined by $\tau_n(\sum_{l=0}^{\infty} z_l t^l) := \sum_{l=0}^{n-1} z_l t^l$ for a positive integer n. In the following argument, we often identify $\zeta_{\mathcal{S}_n}^{\bullet}(\boldsymbol{k})$ with $\tau_n(\zeta_{\widehat{\mathcal{S}}}^{\bullet}(\boldsymbol{k}))$, where $\bullet \in \{\varnothing, \star\}$. Furthermore, we often abbreviate $\zeta(\boldsymbol{k})$ mod $\zeta(2)$ (resp. $\zeta^{ш}(\boldsymbol{k})$ mod $\zeta(2)$) to $\zeta(\boldsymbol{k})$ (resp. $\zeta^{ш}(\boldsymbol{k})$) in $\overline{\mathcal{Z}}$.

THEOREM 3.4. *Let k_1 and k_2 be positive integers. Assume that $k := k_1 + k_2$ is even. Then we have*

$$\zeta_{\mathcal{F}_2}(k_1, k_2) = \frac{1}{2}\left\{(-1)^{k_1} k_2 \binom{k+1}{k_1} - (-1)^{k_2} k_1 \binom{k+1}{k_2} - k\right\} \mathfrak{Z}_{\mathcal{F}_2}(k+1) x_{\mathcal{F}_2}, \tag{3.1}$$

$$\zeta_{\mathcal{F}_2}^{\star}(k_1, k_2) = \frac{1}{2}\left\{(-1)^{k_1} k_2 \binom{k+1}{k_1} - (-1)^{k_2} k_1 \binom{k+1}{k_2} + k\right\} \mathfrak{Z}_{\mathcal{F}_2}(k+1) x_{\mathcal{F}_2}. \tag{3.2}$$

Proof. The case $\mathcal{F} = \mathcal{A}$ was proved by Zhao, see [Zh, Theorem 3.2]. Hereafter, we consider the case $\mathcal{F} = \mathcal{S}$. First, we prove (3.1) for the case $k_1 \geq 2$. By the definition of $\zeta_{\mathcal{S}_2}(k_1, k_2)$, we have

$$\zeta_{\mathcal{S}_2}(k_1, k_2) = \zeta_{\mathcal{S}_1}(k_1, k_2) + \{k_2 \zeta(k_2 + 1, k_1) + k_1 \zeta(k_2, k_1 + 1)\} t.$$

Since $k_1 + k_2$ is even, we have $\zeta_{\mathcal{S}_1}(k_1, k_2) = 0$ by definition. Therefore, by using (2.2), we obtain (3.1) for the case $k_1 \geq 2$. Next, we prove (3.1) for the case $k_1 = 1$ (then k_2 is odd). We have

$$\zeta_{\mathcal{S}_2}(1, k_2) = \{k_2 \zeta^{ш}(k_2 + 1, 1) + \zeta(k_2, 2)\} t. \tag{3.3}$$

By applying Theorem 2.1 for $w = e_1 e_0^{k_2}$ and the sum formula for MZVs of depth 2, we have

$$\zeta^{ш}(k_2+1, 1) = -\zeta(k_2, 2) - \cdots - \zeta(2, k_2) - 2\zeta(1, k_2+1) = -\zeta(k_2+2) - \zeta(1, k_2+1). \tag{3.4}$$

By (2.2), we have

$$\zeta(1, k_2+1) = \frac{k_2+1}{2} \zeta(k_2+2), \quad \zeta(k_2, 2) = \frac{1}{2}\left\{\frac{(k_2+2)(k_2+1)}{2} - 1\right\} \zeta(k_2+2). \tag{3.5}$$

From (3.3), (3.4), (3.5), we obtain (3.1) for the case $k_1 = 1$. The formula (3.2) follows from (3.1), the fact $\zeta_{\mathcal{S}_2}^{\star}(k_1, k_2) = \zeta_{\mathcal{S}_2}(k_1, k_2) + \zeta_{\mathcal{S}_2}(k_1 + k_2)$, and $\zeta_{\mathcal{S}_2}(k) = (-1)^k k \zeta(k+1) t$ (Theorem 3.2 with $\mathcal{F}_n = \mathcal{S}_2$). □

3.3. Depth 3 case

THEOREM 3.5. *Let k_1, k_2, k_3 be positive integers. Suppose that $k := k_1 + k_2 + k_3$ is odd. Then we have*

$$\zeta_{\mathcal{F}_1}(k_1, k_2, k_3) = -\zeta_{\mathcal{F}_1}^{\star}(k_1, k_2, k_3) = \frac{1}{2}\left\{(-1)^{k_1}\binom{k}{k_1} - (-1)^{k_3}\binom{k}{k_3}\right\} \mathfrak{Z}_{\mathcal{F}_1}(k).$$

Proof. The case $\mathcal{F} = \mathcal{A}$ was proved by Hoffman and Zhao; see [H2, Theorem 6.2] or [Zh, Theorem 3.5]. Hereafter, we consider the case $\mathcal{F} = \mathcal{S}$. By Proposition 2.5 and the reversal formula for $\mathcal{F}_1$-MZVs, we have

$$\zeta_{\mathcal{F}_1}^{\star}(k_1, k_2, k_3) = (-1)^{k_1+k_2+k_3} \zeta_{\mathcal{F}_1}(k_1, k_2, k_3) = -\zeta_{\mathcal{F}_1}(k_1, k_2, k_3). \tag{3.6}$$

From

$$\zeta^{\star}_{\mathcal{F}_1}(k_1,k_2,k_3)=\zeta_{\mathcal{F}_1}(k_1,k_2,k_3)+\zeta_{\mathcal{F}_1}(k_1+k_2,k_3)+\zeta_{\mathcal{F}_1}(k_1,k_2+k_3)$$

and the explicit formula for $\mathcal{F}_1$-double zeta values [Kan, (7.2), Example 9.4 (2)], we have

$$\begin{aligned}(3.7)\qquad \zeta_{\mathcal{F}_1}(k_1,k_2,k_3)&=-\frac{\zeta_{\mathcal{F}_1}(k_1+k_2,k_3)+\zeta_{\mathcal{F}_1}(k_1,k_2+k_3)}{2}\\&=-\frac{1}{2}\left\{(-1)^{k_3}\binom{k}{k_1+k_2}+(-1)^{k_2+k_3}\binom{k}{k_1}\right\}\mathfrak{Z}_{\mathcal{F}_1}(k)\\&=\frac{1}{2}\left\{(-1)^{k_1}\binom{k}{k_1}-(-1)^{k_3}\binom{k}{k_3}\right\}\mathfrak{Z}_{\mathcal{F}_1}(k).\end{aligned}$$

The formula for $\zeta^{\star}_{\mathcal{F}_1}(k_1,k_2,k_3)$ is obtained by (3.6) and (3.7). □

3.4. General depth case

THEOREM 3.6. *For positive integers r, k and for $\mathcal{F}\in\{\mathcal{A},\mathcal{S}\}$, we have*

$$(3.8)\qquad \zeta_{\mathcal{F}_2}(\{k\}^r)=(-1)^{r-1}k\mathfrak{Z}_{\mathcal{F}_2}(rk+1)x_{\mathcal{F}_2},$$

$$(3.9)\qquad \zeta^{\star}_{\mathcal{F}_2}(\{k\}^r)=k\mathfrak{Z}_{\mathcal{F}_2}(rk+1)x_{\mathcal{F}_2}.$$

Moreover, we have

$$(3.10)\quad \zeta_{\mathcal{F}_3}(\{k\}^r)=(-1)^{rk+r-1}\Bigg[k\mathfrak{Z}_{\mathcal{F}_3}(rk+1)x_{\mathcal{F}_3}+\left\{\frac{k(rk+1)}{2}\mathfrak{Z}_{\mathcal{F}_3}(rk+2)-k^2\sum_{l=1}^{r-1}\mathfrak{Z}_{\mathcal{F}_3}(lk+1)\mathfrak{Z}_{\mathcal{F}_3}((r-l)k+1)\right\}x^2_{\mathcal{F}_3}\Bigg]$$

and

$$(3.11)\quad \zeta^{\star}_{\mathcal{F}_3}(\{k\}^r)=(-1)^{rk}\Bigg[k\mathfrak{Z}_{\mathcal{F}_3}(rk+1)x_{\mathcal{F}_3}+\left\{\frac{k(rk+1)}{2}\mathfrak{Z}_{\mathcal{F}_3}(rk+2)+k^2\sum_{l=1}^{r-1}\mathfrak{Z}_{\mathcal{F}_3}(lk+1)\mathfrak{Z}_{\mathcal{F}_3}((r-l)k+1)\right\}x^2_{\mathcal{F}_3}\Bigg].$$

REMARK 3.7. If rk is odd, then $\mathfrak{Z}_{\mathcal{F}_3}(rk+1)$ and $\mathfrak{Z}_{\mathcal{F}_3}(lk+1)\mathfrak{Z}_{\mathcal{F}_3}((r-l)k+1)$ are 0, and we have

$$\zeta_{\mathcal{F}_3}(\{k\}^r)=(-1)^r\frac{k(rk+1)}{2}\mathfrak{Z}_{\mathcal{F}_3}(rk+2)x^2_{\mathcal{F}_3},\ \ \zeta^{\star}_{\mathcal{F}_3}(\{k\}^r)=-\frac{k(rk+1)}{2}\mathfrak{Z}_{\mathcal{F}_3}(rk+2)x^2_{\mathcal{F}_3}.$$

These formulas for the case $\mathcal{F}=\mathcal{A}$ were first proved by Zhou and Cai in the last remark of [ZC] but our proof differs from theirs.

Proof. Since (3.8) and (3.9) follows from (3.10) and (3.11) by taking modulo $x^2_{\mathcal{F}_3}$, it is sufficient to prove (3.10) and (3.11). Note that $(-1)^{rk}\mathfrak{Z}_{\mathcal{F}_2}(rk+1)x_{\mathcal{F}_2}=\mathfrak{Z}_{\mathcal{F}_2}(rk+1)x_{\mathcal{F}_2}$ holds because if rk is odd, then $\mathfrak{Z}_{\mathcal{F}_2}(rk+1)x_{\mathcal{F}_2}=0$.

By Theorem 3.2 and the symmetric sum formula (5.1) proved in Section 5 with $\boldsymbol{k} = (\{k\}^r)$, we have

(3.12)

$$\begin{aligned} &r!\zeta_{\mathcal{F}_3}(\{k\}^r) \\ &= (-1)^{rk+r-1}(r-1)!\left\{rk\mathfrak{Z}_{\mathcal{F}_3}(rk+1)x_{\mathcal{F}_3} + \binom{rk+1}{2}\mathfrak{Z}_{\mathcal{F}_3}(rk+2)x_{\mathcal{F}_3}^2\right\} \\ &\quad + (-1)^{rk+r-2}\sum_{\substack{B_1\sqcup B_2=\{1,\dots,r\}\\ B_1,B_2\neq\varnothing}}(\#B_1-1)!(\#B_2-1)!b_1b_2\mathfrak{Z}_{\mathcal{F}_3}(b_1+1)\mathfrak{Z}_{\mathcal{F}_3}(b_2+1)x_{\mathcal{F}_3}^2, \end{aligned}$$

where $b_1 = b_1(\{k\}^r)$ and $b_2 = b_2(\{k\}^r)$ are defined as in Theorem 5.1. Set $l := \#B_1$. Then we see that $1 \le l \le r-1$, $\#B_2 = r-l$, $b_1 = lk$ and $b_2 = (r-l)k$. Moreover, the number of ways of dividing $\{1,\dots,r\}$ into two non-empty subsets B_1 and B_2 with $\#B_1 = l$ is just $\binom{r}{l}$. Therefore, the summation for the partition in the right-hand side of (3.12) coincides with

$$\begin{aligned} &\sum_{l=1}^{r-1}\binom{r}{l}(l-1)!(r-l-1)!\cdot l(r-l)k^2\mathfrak{Z}_{\mathcal{F}_3}(lk+1)\mathfrak{Z}_{\mathcal{F}_3}((r-l)k+1)x_{\mathcal{F}_3}^2 \\ &= k^2\cdot r!\sum_{l=1}^{r-1}\mathfrak{Z}_{\mathcal{F}_3}(lk+1)\mathfrak{Z}_{\mathcal{F}_3}((r-l)k+1)x_{\mathcal{F}_3}^2. \end{aligned}$$

Thus we obtain (3.10). The formula (3.11) is obtained in the same manner. □

THEOREM 3.8. *For non-negative integers a and b, we have*

$$\zeta_{\mathcal{F}_1}(\{1\}^a, 2, \{1\}^b) = (-1)^b\binom{a+b+2}{a+1}\mathfrak{Z}_{\mathcal{F}_1}(a+b+2), \tag{3.13}$$

$$\zeta^\star_{\mathcal{F}_1}(\{1\}^a, 2, \{1\}^b) = (-1)^b\binom{a+b+2}{a+1}\mathfrak{Z}_{\mathcal{F}_1}(a+b+2). \tag{3.14}$$

Proof. The case $\mathcal{F} = \mathcal{A}$ was proved by Hessami-Pilehrood–Hessami-Pilehrood–Tauraso; see [HHT, Theorem 4.5]. Hereafter, we consider the case $\mathcal{F} = \mathcal{S}$. By the definition of $\zeta_{\mathcal{S}_1}(\boldsymbol{k})$ and the fact that $\zeta^{ш}(\{1\}^k) = 0$ for $k \ge 1$, we have

$$\zeta_{\mathcal{S}_1}(\{1\}^a, 2, \{1\}^b) = \zeta^{ш}(\{1\}^a, 2, \{1\}^b) + (-1)^{a+b}\zeta^{ш}(\{1\}^b, 2, \{1\}^a). \tag{3.15}$$

Applying Lemma 2.1 for $w = e_1^{a+1}e_0$ and $m = b$, and using the duality for MZVs, we have

$$\zeta^{ш}(\{1\}^a, 2, \{1\}^b) = (-1)^b\binom{a+b+1}{b}\zeta(a+b+2). \tag{3.16}$$

From (3.15) and (3.16), we obtain (3.13). The formula (3.14) follows from (3.13), Proposition 2.5 and the fact that $\zeta_{\mathcal{S}_1}(\{1\}^r) = \zeta^\star_{\mathcal{S}_1}(\{1\}^r) = 0$ for $r \ge 1$. The last fact is well-known and a special case of Theorem 3.6. □

REMARK 3.9. We can also prove (3.14) using the Hoffman duality ([H2, Theorem 4.6] and [J1, Corollarie 1.12]) and the explicit formula for $\zeta_{\mathcal{F}_1}(a+1, b+1)$.

THEOREM 3.10. *For non-negative integers a and b, we have*

$$\zeta_{\mathcal{F}_1}(\{2\}^a, 3, \{2\}^b) = \frac{(-1)^{a+b}2(a-b)}{a+1}\binom{2a+2b+3}{2b+2}\mathfrak{Z}_{\mathcal{F}_1}(2a+2b+3), \tag{3.17}$$

$$\zeta^\star_{\mathcal{F}_1}(\{2\}^a, 3, \{2\}^b) = \frac{2(b-a)}{a+1}\binom{2a+2b+3}{2b+2}\mathfrak{Z}_{\mathcal{F}_1}(2a+2b+3). \tag{3.18}$$

Proof. The case $\mathcal{F} = \mathcal{A}$ was proved by Hessami-Pilehrood–Hessami-Pilehrood–Tauraso; see [HHT, Theorem 4.1]. Hereafter, we consider the case $\mathcal{F} = \mathcal{S}$. By the definition of the $\mathcal{S}_1$-MZV and the fact that $\zeta(\{2\}^r) \equiv 0 \pmod{\zeta(2)}$ for $r \geq 1$, we have

$$\zeta_{\mathcal{S}_1}(\{2\}^a, 3, \{2\}^b) = \zeta(\{2\}^a, 3, \{2\}^b) - \zeta(\{2\}^b, 3, \{2\}^a).$$

Thus we obtain (3.17) by the formula (2.1) and straightforward calculation of binomial coefficients. The formula (3.18) is obtained by (3.17), Proposition 2.5 and a special case of Theorem 3.6, that is, the fact that $\zeta_{\mathcal{S}_1}(\{2\}^r) = \zeta^\star_{\mathcal{S}_1}(\{2\}^r) = 0$ for $r \geq 1$. □

THEOREM 3.11. *For non-negative integers a and b, we have*

(3.19)

$$\zeta_{\mathcal{F}_1}(\{2\}^a, 1, \{2\}^b) = 4(-1)^{a+b}\frac{a-b}{2a+1}\left(1 - \frac{1}{4^{a+b}}\right)\binom{2a+2b+1}{2b+1}\mathfrak{Z}_{\mathcal{F}_1}(2a+2b+1),$$

(3.20)

$$\zeta^\star_{\mathcal{F}_1}(\{2\}^a, 1, \{2\}^b) = \frac{4(b-a)}{2a+1}\left(1 - \frac{1}{4^{a+b}}\right)\binom{2a+2b+1}{2b+1}\mathfrak{Z}_{\mathcal{F}_1}(2a+2b+1).$$

Proof. The case $\mathcal{F} = \mathcal{A}$ was proved by Hessami-Pilehrood–Hessami-Pilehrood–Tauraso; see [HHT, Theorem 4.2]. Hereafter, we consider the case $\mathcal{F} = \mathcal{S}$. First, we prove (3.19) for the case $a, b \geq 1$. By the definition of the $\mathcal{S}_1$-MZV and the duality for MZVs, we obtain

$$\zeta_{\mathcal{S}_1}(\{2\}^a, 1, \{2\}^b) = \zeta(\{2\}^{b-1}, 3, \{2\}^a) - \zeta(\{2\}^{a-1}, 3, \{2\}^b).$$

Then we obtain (3.19) by a similar calculation in Theorem 3.10 using (2.1).

Next we prove (3.19) for the case $a \geq 1$ and $b = 0$. We have

$$\zeta_{\mathcal{S}_1}(\{2\}^a, 1) = \zeta^{Ш}(\{2\}^a, 1) - \zeta(1, \{2\}^a). \tag{3.21}$$

Applying Lemma 2.1 for $w = (e_1e_0)^a$ and $m = 1$, we obtain

$$\zeta^{Ш}(\{2\}^a, 1) = -2\sum_{j=0}^{a-1}\zeta(\{2\}^j, 1, \{2\}^{a-j}).$$

Thus, by the duality for MZVs, we have

$$\begin{aligned}\zeta_{\mathcal{S}_1}(\{2\}^a, 1) &= -\zeta(1, \{2\}^a) - 2\sum_{j=0}^{a-1}\zeta(\{2\}^j, 1, \{2\}^{a-j}) \\ &= -\zeta(\{2\}^{a-1}, 3) - 2\sum_{j=0}^{a-1}\zeta(\{2\}^{a-j-1}, 3, \{2\}^j).\end{aligned} \tag{3.22}$$

By (2.1), we obtain

$$\zeta(\{2\}^{a-j-1}, 3, \{2\}^j) = 2(-1)^a \left\{ \binom{2a}{2j} - \left(1 - \frac{1}{4^a}\right) \binom{2a}{2j+1} \right\} \zeta(2a+1) \tag{3.23}$$

for $0 \le j \le a-1$. Therefore, from (3.22) and (3.23), we obtain (3.19) for the case $a \ge 1$ and $b = 0$. The case $a = 0$ and $b \ge 1$ of (3.19) follows easily from the reversal formula and (3.22) with $a \ge 1$. This completes the proof of (3.19). The formula (3.20) is obtained by (3.19), Proposition 2.5 and the fact that $\zeta_{\mathcal{S}_1}(\{2\}^r) = \zeta^\star_{\mathcal{S}_1}(\{2\}^r) = 0$ for $r \ge 1$. □

REMARK 3.12. Tasaka and Yamamoto proved an analogous formula of Theorem 2.2 for $\zeta^\star(\{2\}^a, 1, \{2\}^b)$; see [TY, Theorem 1.6]. We can also obtain Theorem 3.11 by a similar approach using [TY, Theorem 1.6] and Proposition 2.5 instead of Zagier's formula (Theorem 2.2).

The following theorem is a refinement of the even weight case in Theorem 3.8.

THEOREM 3.13. *Let a and b be non-negative integers. Assume that a + b is even. Then we have*

$$\zeta_{\mathcal{F}_2}(\{1\}^a, 2, \{1\}^b) = \frac{1}{2}\left\{1 + (-1)^a \binom{a+b+3}{b+2}\right\} \mathfrak{z}_{\mathcal{F}_2}(a+b+3) x_{\mathcal{F}_2}, \tag{3.24}$$

$$\zeta^\star_{\mathcal{F}_2}(\{1\}^a, 2, \{1\}^b) = \frac{1}{2}\left\{1 + (-1)^a \binom{a+b+3}{a+2}\right\} \mathfrak{z}_{\mathcal{F}_2}(a+b+3) x_{\mathcal{F}_2}. \tag{3.25}$$

Proof. The case $\mathcal{F} = \mathcal{A}$ was proved by Hessami-Pilehrood–Hessami-Pilehrood–Tauraso [HHT, Theorem 4.5]; there is also another proof by Sakugawa and the third author [SS, Theorem 3.18]. Hereafter, we consider the case $\mathcal{F} = \mathcal{S}$. We first prove the formula (3.24). Set $d := a+b+1$ and $\boldsymbol{k} = (k_1, \dots, k_d) := (\{1\}^a, 2, \{1\}^b)$. For $0 \le i \le d$, we set

$$P_i(t) := (-1)^{k_{i+1}+\cdots+k_d} \zeta^{Ш}(k_1, \dots, k_i) \times \sum_{\substack{l_{i+1},\dots,l_d \ge 0 \\ l_{i+1}+\cdots+l_d \le 1}} \left[\prod_{j=i+1}^{d} \binom{k_j + l_j - 1}{l_j}\right] \zeta^{Ш}(k_d + l_d, \dots, k_{i+1} + l_{i+1}) t^{l_{i+1}+\cdots+l_d}.$$

Note that this expression for the case $i = d$ means $P_d(t) = \zeta^{Ш}(\boldsymbol{k})$. Then, by the definition of $\zeta_{\mathcal{S}_2}(\boldsymbol{k})$, we have

$$\zeta_{\mathcal{S}_2}(\boldsymbol{k}) = \sum_{i=0}^{d} P_i(t).$$

We prove that for $1 \le i \le a+b+1$, $P_i(t) = 0$ in $\overline{\mathcal{Z}}[t]$. Since $\zeta^{Ш}(\{1\}^k) = 0$ for a positive integer k, we obtain $P_1(t) = \cdots = P_a(t) = 0$. For $0 \le j \le b$, we calculate $P_{a+j+1}(t)$. By the definition of $P_i(t)$, we have

$$P_{a+j+1}(t) = (-1)^{b-j} \zeta^{Ш}(\{1\}^a, 2, \{1\}^j) \left(\zeta^{Ш}(\{1\}^{b-j}) + \sum_{i=1}^{b-j} \zeta^{Ш}(\{1\}^{i-1}, 2, \{1\}^{b-j-i}) t \right).$$

By (3.16), we have $\zeta^{ш}(\{1\}^a, 2, \{1\}^j) = (-1)^j \binom{a+j+1}{j} \zeta(a+j+2)$. Since $\zeta(a+b+2) = 0$ in $\overline{\mathcal{Z}}$, we have $P_{a+b+1}(t) = 0$ in $\overline{\mathcal{Z}}[t]$. Assume that $j < b$. In this case, $\zeta^{ш}(\{1\}^{b-j}) = 0$ holds. By the shuffle-regularized sum formula [Li, Lemma 3.3] (or [KS, Theorem 1.2]), and the duality for MZVs, we have

$$\sum_{i=1}^{b-j} \zeta^{ш}(\{1\}^{i-1}, 2, \{1\}^{b-j-i}) = (-1)^{b-j-1} \zeta(b-j+1).$$

Since $a+b$ is even, $a+j+2 \not\equiv b-j+1 \pmod 2$ and thus we have $P_{a+j+1}(t) = 0$ in $\overline{\mathcal{Z}}$.

The calculation of $P_0(t)$ remains. State $P_0(t) = A + Bt$ with $A, B \in \overline{\mathcal{Z}}$. Then from (3.16), we have $A = \zeta^{ш}(\{1\}^b, 2, \{1\}^a) = 0$ in $\overline{\mathcal{Z}}$. By definition, B is expressed as follows:

$$\begin{aligned} B = &\sum_{\substack{l+m=b-1 \\ l,m\geq 0}} \zeta^{ш}(\{1\}^l, 2, \{1\}^m, 2, \{1\}^a) \\ &+ 2\zeta^{ш}(\{1\}^b, 3, \{1\}^a) + \sum_{\substack{m+n=a-1 \\ m,n\geq 0}} \zeta^{ш}(\{1\}^b, 2, \{1\}^m, 2, \{1\}^n). \end{aligned}$$

For general non-negative integers l, m and n, by the regularization formula (Lemma 2.1), we have

$$\zeta^{ш}(\{1\}^l, 2, \{1\}^m, 2, \{1\}^n) = (-1)^n \sum_{\substack{r+s=n \\ r,s\geq 0}} \binom{r+l+1}{r}\binom{s+m+1}{s} \zeta(\{1\}^{r+l}, 2, \{1\}^{s+m}, 2),$$

$$\zeta^{ш}(\{1\}^l, 3, \{1\}^n) = (-1)^n \sum_{\substack{r+s=n \\ r,s\geq 0}} \binom{r+l+1}{r} \zeta(\{1\}^{r+l}, 2, \{1\}^{s-1}, 2),$$

where $\zeta(\{1\}^{r+l}, 2, \{1\}^{-1}, 2)$ means $\zeta(\{1\}^{r+l}, 3)$. Thus, with the duality for MZVs, we obtain

$$\begin{aligned} B = &\sum_{\substack{l+m=b-1 \\ l,m\geq 0}} (-1)^a \sum_{\substack{r+s=a \\ r,s\geq 0}} \binom{r+l+1}{r}\binom{s+m+1}{s} \zeta(s+m+2, r+l+2) \\ &+ 2(-1)^a \sum_{\substack{r+s=a \\ r,s\geq 0}} \binom{r+b+1}{r} \zeta(s+1, r+b+2) \\ &+ \sum_{\substack{m+n=a-1 \\ m,n\geq 0}} (-1)^n \sum_{\substack{r+s=n \\ r,s\geq 0}} \binom{r+b+1}{r}\binom{s+m+1}{s} \zeta(s+m+2, r+b+2). \end{aligned}$$

Since $a+b+3$ is odd, by using (2.2), we can rewrite B as a rational multiple of the Riemann zeta value $\zeta(a+b+3)$. Specifically, we have $B = \frac{1}{2}C\zeta(a+b+3)$ with

$$C = \sum_{\substack{l+m=b-1 \\ l,m\geq 0}} (-1)^a \sum_{\substack{r+s=a \\ r,s\geq 0}} \binom{r+l+1}{r}\binom{s+m+1}{s} (-1)^{s+m+1} \left\{ \binom{a+b+3}{s+m+2} + (-1)^{s+m} \right\}$$

$$+2(-1)^a \sum_{\substack{r+s=a\\ r,s\geq 0}} \binom{r+b+1}{r}(-1)^s \left\{\binom{a+b+3}{s+1} + (-1)^{s+1}\right\}$$
$$+ \sum_{\substack{m+n=a-1\\ m,n\geq 0}} (-1)^n \sum_{\substack{r+s=n\\ r,s\geq 0}} \binom{r+b+1}{r}\binom{s+m+1}{s}(-1)^{s+m+1}\left\{\binom{a+b+3}{s+m+2}+(-1)^{s+m}\right\}.$$

Therefore, it suffices to prove the following:

$$C = 1 + (-1)^a \binom{a+b+3}{b+2}. \tag{3.26}$$

We prove this in the Appendix. From this, we obtain the desired formula for $\zeta_{\mathcal{S}_2}(\{1\}^a, 2, \{1\}^b)$.

Next, we prove (3.25). By Proposition 2.5, we have

$$\zeta^{\star}_{\mathcal{S}_2}(\{1\}^a, 2, \{1\}^b) - \zeta_{\mathcal{S}_2}(\{1\}^b, 2, \{1\}^a) = \sum_{j=1}^{a}(-1)^j \zeta_{\mathcal{S}_2}(\{1\}^b, 2, \{1\}^{a-j})\zeta^{\star}_{\mathcal{S}_2}(\{1\}^j)$$
$$+ \sum_{i=1}^{b}(-1)^{b-i} \zeta_{\mathcal{S}_2}(\{1\}^{b+1-i})\zeta^{\star}_{\mathcal{S}_2}(\{1\}^a, 2, \{1\}^{i-1}).$$

It is sufficient to show that the right-hand side vanishes. If j is odd, then we have $\zeta^{\star}_{\mathcal{S}_2}(\{1\}^j) = 0$ by (3.9). If j is even, then both $\zeta^{\star}_{\mathcal{S}_2}(\{1\}^j)$ and $\zeta_{\mathcal{S}_2}(\{1\}^b, 2, \{1\}^{a-j})$ can be seen as elements of $t\overline{\mathcal{Z}}[t]$ by (3.9) and (3.13). Thus the first summation vanishes in $\overline{\mathcal{Z}}[\![t]\!]/(t^2)$. Similarly, if $b-i$ is even, then we have $\zeta_{\mathcal{S}_2}(\{1\}^{b+1-i}) = 0$ by (3.8). If $b-i$ is odd, then both $\zeta_{\mathcal{S}_2}(\{1\}^{b+1-i})$ and $\zeta^{\star}_{\mathcal{S}_2}(\{1\}^a, 2, \{1\}^{i-1})$ can be seen as elements of $t\overline{\mathcal{Z}}[t]$ by (3.8) and (3.14). Therefore, the second summation also vanishes. □

REMARK 3.14. The proof of the case $\mathcal{F} = \mathcal{A}$ of Theorem 3.13 by Sakugawa and the third author is based on the '$\mathcal{A}_2$-duality' [SS, Remark 3.14 (40)]. If the '$\mathcal{S}_2$-duality' is established, then we can obtain another proof of the case $\mathcal{F} = \mathcal{S}$ of Theorem 3.13. When we were writing this paper, a preprint [TT] by Takeyama and Tasaka appeared on arXiv. Their [TT, Corollary 6.8] contains the $\mathcal{S}_2$-duality as a special case.

4. Bowman–Bradley type theorem

Murahara, Onozuka and the third author [MOS] proved the Bowman–Bradley type theorem for $\mathcal{A}_2$-MZ(S)Vs (= the case $\mathcal{F} = \mathcal{A}$ of Theorem 4.1). In this section, we prove the $\mathcal{S}_2$-counterpart of their theorem. By combining these two theorems, we have the following.

THEOREM 4.1 (Bowman–Bradley type theorem for $\mathcal{F}_2$-MZ(S)V). *For non-negative integers l and m with $(l, m) \neq (0, 0)$, we have*

$$\begin{aligned}(4.1)\quad &\sum_{\substack{m_0+\cdots+m_{2l}=m\\ m_0,\ldots,m_{2l}\geq 0}} \zeta_{\mathcal{F}_2}\big(\{2\}^{m_0}, 1, \{2\}^{m_1}, 3, \{2\}^{m_2}, \ldots, \{2\}^{m_{2l-2}}, 1, \{2\}^{m_{2l-1}}, 3, \{2\}^{m_{2l}}\big)\\ &= (-1)^m \left\{(-1)^l 2^{1-2l}\binom{l+m}{l} - 4\binom{2l+m}{2l}\right\} \mathfrak{z}_{\mathcal{F}_2}(4l+2m+1)x_{\mathcal{F}_2},\end{aligned}$$

$$\begin{aligned}(4.2)\quad &\sum_{\substack{m_0+\cdots+m_{2l}=m\\ m_0,\ldots,m_{2l}\geq 0}} \zeta^{\star}_{\mathcal{F}_2}\big(\{2\}^{m_0}, 1, \{2\}^{m_1}, 3, \{2\}^{m_2}, \ldots, \{2\}^{m_{2l-2}}, 1, \{2\}^{m_{2l-1}}, 3, \{2\}^{m_{2l}}\big)\\ &= (-1)^l 2^{1-2l}\binom{l+m}{l} \mathfrak{z}_{\mathcal{F}_2}(4l+2m+1)x_{\mathcal{F}_2}.\end{aligned}$$

This gives a partial lift of the Bowman–Bradley type theorem for $\mathcal{F}_1$-MZ(S)V proved by Saito and Wakabayashi [SW2]. Note that the proof of the $\mathcal{F} = \mathcal{S}$ case in Theorem 4.1 presented here is essentially the same as the proof of the $\mathcal{F} = \mathcal{A}$ case by Murahara, Onozuka and the third author [MOS]. In contrast, proofs of some sum formulas which will be given in the next section are different from those in the previous study.

We prepare two lemmas for the proof.

LEMMA 4.2. *For non-negative integers l and m with $(l, m) \neq (0, 0)$, we have*

$$Z_{\mathcal{S}_2}\big(e_2^{l+m} ш e_2^{l}\big) = (-1)^m 2\left\{1 - 2\binom{4l+2m}{2l}\right\}\zeta(4l+2m+1)t.$$

Proof. This lemma is the $\mathcal{S}_2$-counterpart of [MOS, Lemma 2.5] and is proved from the same argument in [MOS] by using the explicit evaluation of $\zeta_{\mathcal{S}_2}(\{2\}^r)$ ((3.8) with $k = 2$), (3.17) and (2.4) with $\mathcal{F}_n = \mathcal{S}_2$. □

For a positive integer n, define a $\mathbb{Q}$-linear map $Z^{\star}_{\mathcal{S}_n} : \mathfrak{H}^1 \to \overline{\mathcal{Z}}[[t]]/(t^n)$ by $Z^{\star}_{\mathcal{S}_n}(e_{\boldsymbol{k}}) := \zeta^{\star}_{\mathcal{S}_n}(\boldsymbol{k})$ for any index $\boldsymbol{k}$.

LEMMA 4.3. *For non-negative integers l and m, we have*

$$\begin{aligned}&Z^{\star}_{\mathcal{S}_2}\big((e_1e_3)^l \,\widetilde{ш}\, e_2^m\big)\\ &= \sum_{\substack{2i+k+u=2l\\ j+n+v=m}} (-1)^{j+k}\binom{k+n}{k}\binom{u+v}{u} Z_{\mathcal{S}_2}\big((e_1e_3)^i \,\widetilde{ш}\, e_2^j\big)Z^{\star}_{\mathcal{S}_2}\big(e_2^{k+n}\big)Z^{\star}_{\mathcal{S}_2}\big(e_2^{u+v}\big).\end{aligned}$$

Proof. This follows immediately from [Y, equation (3.1)] and (2.3) with $\mathcal{F}_n = \mathcal{S}_2$. □

Proof of the $\mathcal{F} = \mathcal{S}$ case in Theorem 4.1. We prove (4.1) by induction on $l \geq 0$. The case $l = 0$ holds by the explicit evaluation of $\zeta_{\mathcal{S}_2}(\{2\}^r)$ ((3.8) with $k = 2$). Let l be a positive integer and m a non-negative integer. By [MOS, Lemma 2.1], we have

$$Z_{\mathcal{S}_2}\big((e_1e_3)^l \,\widetilde{ш}\, e_2^m\big)$$

$$= 4^{-l} Z_{\mathcal{S}_2}\big(e_2^{l+m} \text{ Ш } e_2^{l}\big) - \sum_{k=0}^{l-1} 4^{k-l} \binom{2l+m-2k}{l-k} Z_{\mathcal{S}_2}\big((e_1e_3)^k \,\widetilde{\text{Ш}}\, e_2^{2l+m-2k}\big).$$

Hence, by Lemma 4.2 and the induction hypothesis, we have

$$\begin{aligned} &Z_{\mathcal{S}_2}\big((e_1e_3)^l \,\widetilde{\text{Ш}}\, e_2^m\big) \\ &= (-1)^m 2^{1-2l} \left\{1 - 2\binom{4l+2m}{2l}\right\} \zeta(4l+2m+1)t \\ &\quad - \sum_{k=0}^{l-1} 4^{k-l} \binom{2l+m-2k}{l-k} \\ &\quad \cdot (-1)^m \left\{(-1)^k 2^{1-2k} \binom{2l+m-k}{k} - 4\binom{2l+m}{2k}\right\} \zeta(4l+2m+1)t \bmod \zeta(2). \end{aligned}$$

We see that this coincides with the desired formula by using [MOS, Lemma 2.6]. We also obtain (4.2) by the same argument in [MOS] using (4.1), (3.9) with $k = 2$ and Lemma 4.3. □

5. Sum formulas

In this section, we prove the *$\mathcal{F}_n$-symmetric sum formula* (= Theorem 5.1), the *$\mathcal{F}_n$-sum formula over $I_{k,r}$* for $n = 2, 3$ (= Theorem 5.2), and the *$\mathcal{F}_2$-sum formula over $I_{k,r,i}$* (= Theorem 5.4).

5.1. $\mathcal{F}_n$-symmetric sum formula

We first state the $\mathcal{F}_n$-symmetric sum formula.

THEOREM 5.1 ($\mathcal{F}_n$-symmetric sum formula). *Let n and r be positive integers and $\boldsymbol{k} = (k_1, \dots, k_r)$ an index. Then, we have*

$$\sum_{\sigma\in\mathfrak{S}_r} \zeta_{\mathcal{F}_n}(\sigma(\boldsymbol{k})) = \sum_{\mathcal{B}=\{B_1,\dots,B_l\}} (-1)^{r-l} c(\mathcal{B}) \zeta_{\mathcal{F}_n}(b_1(\boldsymbol{k})) \cdots \zeta_{\mathcal{F}_n}(b_l(\boldsymbol{k})), \tag{5.1}$$

$$\sum_{\sigma\in\mathfrak{S}_r} \zeta^{\star}_{\mathcal{F}_n}(\sigma(\boldsymbol{k})) = \sum_{\mathcal{B}=\{B_1,\dots,B_l\}} c(\mathcal{B}) \zeta_{\mathcal{F}_n}(b_1(\boldsymbol{k})) \cdots \zeta_{\mathcal{F}_n}(b_l(\boldsymbol{k})). \tag{5.2}$$

Here, $\mathfrak{S}_r$ denotes the symmetric group of degree r. For $\sigma \in \mathfrak{S}_r$, set $\sigma(\boldsymbol{k}) := (k_{\sigma(1)}, \dots, k_{\sigma(r)})$. $\mathcal{B} = \{B_1, \dots, B_l\}$ runs all partitions of $\{1, \dots, r\}$, that is, $\mathcal{B} = \{B_1, \dots, B_l\}$ satisfies that $\{1, \dots, r\} = \bigsqcup_{i=1}^{l} B_i$ and $B_i \neq \varnothing$ $(1 \le i \le l)$. Moreover, we set $c(\mathcal{B}) := (\#B_1 - 1)! \cdots (\#B_l - 1)!$ and $b_i(\boldsymbol{k}) := \sum_{j\in B_i} k_j$.

Proof. Since $\mathcal{F}_n$-MZVs satisfy the harmonic relation (2.3), we see that the desired formulas hold by the same argument as [H2, Theorem 4.1]. □

5.2. $\mathcal{F}_n$-sum formula over $I_{k,r}$ for $n = 2, 3$

Next, we prove the $\mathcal{F}_n$-sum formula over $I_{k,r}$ for $n = 2, 3$. For positive integers n, r and k with $r \le k$, $\mathcal{F} \in \{\mathcal{A}, \mathcal{S}\}$ and $\bullet \in \{\varnothing, \star\}$, set

$$S^{\bullet}_{\mathcal{F}_n;k,r} := \sum_{\boldsymbol{k} \in I_{k,r}} \zeta^{\bullet}_{\mathcal{F}_n}(\boldsymbol{k}),$$

where $I_{k,r}$ denotes the set of all indices $\boldsymbol{k}$ with $\mathrm{wt}(\boldsymbol{k}) = k$ and $\mathrm{dep}(\boldsymbol{k}) = r$.

THEOREM 5.2 ($\mathcal{F}_n$-sum formula over $I_{k,r}$ for $n = 2, 3$). *For positive integers r and k with $r \le k$, we have*

$$S_{\mathcal{F}_2;k,r} = (-1)^{r-1}\binom{k}{r}\mathfrak{z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2}, \quad S^{\star}_{\mathcal{F}_2;k,r} = \binom{k}{r}\mathfrak{z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2}. \tag{5.3}$$

Moreover, we have

$$S_{\mathcal{F}_3;k,r} = (-1)^{k+r-1}\left[\binom{k}{r}\mathfrak{z}_{\mathcal{F}_3}(k+1)x_{\mathcal{F}_3} + \left\{\frac{k+1}{2}\binom{k}{r}\mathfrak{z}_{\mathcal{F}_3}(k+2) - \frac{1}{r!}\cdot T_{k,r}\right\}x^2_{\mathcal{F}_3}\right] \tag{5.4}$$

and

$$S^{\star}_{\mathcal{F}_3;k,r} = (-1)^{k}\left[\binom{k}{r}\mathfrak{z}_{\mathcal{F}_3}(k+1)x_{\mathcal{F}_3} + \left\{\frac{k+1}{2}\binom{k}{r}\mathfrak{z}_{\mathcal{F}_3}(k+2) + \frac{1}{r!}\cdot T_{k,r}\right\}x^2_{\mathcal{F}_3}\right], \tag{5.5}$$

where

$$T_{k,r} = \sum_{\substack{B_1 \sqcup B_2 = \{1,\dots,r\} \\ B_1, B_2 \neq \varnothing}} \sum_{\substack{b_1+b_2=k \\ b_1 \ge \#B_1, b_2 \ge \#B_2}} (b_1)_{\#B_1}(b_2)_{\#B_2} \cdot \mathfrak{z}_{\mathcal{F}_3}(b_1+1)\mathfrak{z}_{\mathcal{F}_3}(b_2+1)$$

and the symbol $(n)_m$ denotes $n(n-1)\cdots(n-m+1)$.

REMARK 5.3. If $k = b_1 + b_2$ is odd, since $\mathfrak{z}_{\mathcal{F}_3}(k+1)$ and $\mathfrak{z}_{\mathcal{F}_3}(b_1+1)\mathfrak{z}_{\mathcal{F}_3}(b_2+1)$ are 0, we have

$$S_{\mathcal{F}_3;k,r} = (-1)^r\frac{k+1}{2}\binom{k}{r}\mathfrak{z}_{\mathcal{F}_3}(k+2)x^2_{\mathcal{F}_3}, \quad S^{\star}_{\mathcal{F}_3;k,r} = -\frac{k+1}{2}\binom{k}{r}\mathfrak{z}_{\mathcal{F}_3}(k+2)x^2_{\mathcal{F}_3},$$

which were first proved by the third author and Yamamoto [SY, Theorem 2.5] for $\mathcal{F} = \mathcal{A}$.

Proof of Theorem 5.2. Since (5.3) is obtained from (5.4) and (5.5) by taking modulo $x^2_{\mathcal{F}_3}$, it is sufficient to prove (5.4) and (5.5). Note that $(-1)^k\mathfrak{z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2} = \mathfrak{z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2}$ holds because if k is odd, then $\mathfrak{z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2} = 0$.

Let us prove (5.4). By Theorem 3.2, we have

$$\zeta_{\mathcal{F}_3}(k) = (-1)^k\left\{k\mathfrak{z}_{\mathcal{F}_3}(k+1)x_{\mathcal{F}_3} + \binom{k+1}{2}\mathfrak{z}_{\mathcal{F}_3}(k+2)x^2_{\mathcal{F}_3}\right\}. \tag{5.6}$$

Since $x^l_{\mathcal{F}_3}$ with $l \ge 3$ vanishes, by (5.1), we have

$$\begin{aligned} S_{\mathcal{F}_3;k,r} &= \frac{1}{r!}\sum_{\boldsymbol{k} \in I_{k,r}}\sum_{\sigma \in \mathfrak{S}_r}\zeta_{\mathcal{F}_3}(\sigma(\boldsymbol{k})) \\ &= \frac{1}{r!}\sum_{\boldsymbol{k} \in I_{k,r}}\Big\{(-1)^{r-1}(r-1)!\zeta_{\mathcal{F}_3}(k) \end{aligned}$$

$$+(-1)^{r-2}\sum_{\substack{B_1\sqcup B_2=\{1,\dots,r\}\\ B_1,B_2\neq\varnothing}}(\#B_1-1)!(\#B_2-1)!\zeta_{\mathcal{F}_3}(b_1(\boldsymbol{k}))\zeta_{\mathcal{F}_3}(b_2(\boldsymbol{k}))\Bigg\}.$$

We calculate the right-hand side. Since $\#I_{k,r}=\binom{k-1}{r-1}$, by (5.6), we have

$$\sum_{\boldsymbol{k}\in I_{k,r}}\frac{(-1)^{r-1}}{r}\zeta_{\mathcal{F}_3}(\boldsymbol{k})=(-1)^{k+r-1}\left\{\binom{k}{r}\mathfrak{Z}_{\mathcal{F}_3}(k+1)x_{\mathcal{F}_3}+\frac{k+1}{2}\binom{k}{r}\mathfrak{Z}_{\mathcal{F}_3}(k+2)x_{\mathcal{F}_3}^2\right\}.$$

Furthermore, since $\#\{\boldsymbol{k}=(k_1,\dots,k_r)\in I_{k,r}\mid\sum_{i\in B_1}k_i=b_1\}=\#I_{b_1,\#B_1}\cdot\#I_{b_2,\#B_2}$ for $B_1,B_2\neq\varnothing$ with $B_1\sqcup B_2=\{1,\dots,r\}$ and b_1,b_2 with $b_1+b_2=k$, $b_1\geq\#B_1$, $b_2\geq\#B_2$, we have

$$\begin{aligned}&\sum_{\boldsymbol{k}\in I_{k,r}}\sum_{\substack{B_1\sqcup B_2=\{1,\dots,r\}\\ B_1,B_2\neq\varnothing}}(\#B_1-1)!(\#B_2-1)!\zeta_{\mathcal{F}_3}(b_1(\boldsymbol{k}))\zeta_{\mathcal{F}_3}(b_2(\boldsymbol{k}))\\&=\sum_{\substack{B_1\sqcup B_2=\{1,\dots,r\}\\ B_1,B_2\neq\varnothing}}\sum_{\substack{b_1+b_2=k\\ b_1\geq\#B_1,b_2\geq\#B_2}}\sum_{\substack{\boldsymbol{k}=(k_1,\dots,k_r)\in I_{k,r}\\ \sum_{i\in B_1}k_i=b_1}}(\#B_1-1)!(\#B_2-1)!\zeta_{\mathcal{F}_3}(b_1)\zeta_{\mathcal{F}_3}(b_2)\\&=(-1)^k\sum_{\substack{B_1\sqcup B_2=\{1,\dots,r\}\\ B_1,B_2\neq\varnothing}}\sum_{\substack{b_1+b_2=k\\ b_1\geq\#B_1,b_2\geq\#B_2}}(b_1)_{\#B_1}(b_2)_{\#B_2}\cdot\mathfrak{Z}_{\mathcal{F}_3}(b_1+1)\mathfrak{Z}_{\mathcal{F}_3}(b_2+1)x_{\mathcal{F}_3}^2.\end{aligned}$$

Note that all terms of $x_{\mathcal{F}_3}^l$ with $l\geq 3$ for $\mathcal{F}_3$-MZVs vanish. This completes the calculation for (5.4). The formula (5.5) is obtained by a similar calculation using (5.2). □

5.3. $\mathcal{F}_2$-sum formula over $I_{k,r,i}$

In this subsection, we prove the $\mathcal{F}_2$-sum formula over $I_{k,r,i}$. For positive integers k,r,i with $1\leq i\leq r<k$, let $I_{k,r,i}$ denote the set of indices $\boldsymbol{k}=(k_1,\dots,k_r)$ with $\mathrm{wt}(\boldsymbol{k})=k$, $\mathrm{dep}(\boldsymbol{k})=r$ and $k_i\geq 2$. For $\bullet\in\{\varnothing,\star\}$ and a positive integer n, set

$$S^{\bullet}_{\mathcal{F}_n;k,r,i}:=\sum_{\boldsymbol{k}\in I_{k,r,i}}\zeta^{\bullet}_{\mathcal{F}_n}(\boldsymbol{k}).$$

Saito and Wakabayashi [SW1] ($\mathcal{F}=\mathcal{A}$) and Murahara [Mur] ($\mathcal{F}=\mathcal{S}$) proved that

$$S_{\mathcal{F}_1;k,r,i}=(-1)^i\left\{\binom{k-1}{i-1}+(-1)^r\binom{k-1}{r-i}\right\}\mathfrak{Z}_{\mathcal{F}_1}(k),$$
$$S^{\star}_{\mathcal{F}_1;k,r,i}=(-1)^i\left\{\binom{k-1}{r-i}+(-1)^r\binom{k-1}{i-1}\right\}\mathfrak{Z}_{\mathcal{F}_1}(k).$$

If k is even, then we have $S_{\mathcal{F}_1;k,r,i}=S^{\star}_{\mathcal{F}_1;k,r,i}=0$ by $\mathfrak{Z}_{\mathcal{F}_1}(k)=0$. Thus it is a natural question what is a lifting of $S^{\bullet}_{\mathcal{F}_1;k,r,i}$ to $\mathcal{F}_2$, that is, $S^{\bullet}_{\mathcal{F}_2;k,r,i}$. We give the answer in the following form.

THEOREM 5.4 ($\mathcal{F}_2$-sum formula for $I_{k,r,i}$). *Let k,r,i be positive integers with $1\leq i\leq r<k$ and suppose that k is even. Then we have*

$$S_{\mathcal{F}_2;k,r,i}=(-1)^{r-1}\frac{b_{k,r,i}}{2}\cdot\mathfrak{Z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2},\quad S^{\star}_{\mathcal{F}_2;k,r,i}=\frac{b^{\star}_{k,r,i}}{2}\cdot\mathfrak{Z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2},$$

where

$$b_{k,r,i} \coloneqq \binom{k-1}{r} + (-1)^{r-i}\left\{(k-r)\binom{k}{i-1} + \binom{k-1}{i-1} + (-1)^{r-1}\binom{k-1}{r-i}\right\}$$

and

$$b^{\star}_{k,r,i} \coloneqq \binom{k-1}{r} + (-1)^{i-1}\left\{(k-r)\binom{k}{r-i} + \binom{k-1}{r-i} + (-1)^{r-1}\binom{k-1}{i-1}\right\}.$$

The case $\mathcal{F} = \mathcal{A}$ of Theorem 5.4 was proved by the third author and Yamamoto [SY]. In this subsection, we reprove their result and prove the case $\mathcal{F} = \mathcal{S}$ simultaneously by a different method.

LEMMA 5.5 (Recurrence relations). *For positive integers k, r, i with $2 \le i+1 \le r \le k-1$, we have*

$$(r-i)S_{\mathcal{F}_2;k,r,i} + iS_{\mathcal{F}_2;k,r,i+1} + (k-r)S_{\mathcal{F}_2;k,r-1,i} = \sum_{l=1}^{k-r} \zeta_{\mathcal{F}_2}(l) S_{\mathcal{F}_2;k-l,r-1,i},$$

$$(r-i)S^{\star}_{\mathcal{F}_2;k,r,i} + iS^{\star}_{\mathcal{F}_2;k,r,i+1} - (k-r)S^{\star}_{\mathcal{F}_2;k,r-1,i} = \sum_{l=1}^{k-r} \zeta_{\mathcal{F}_2}(l) S^{\star}_{\mathcal{F}_2;k-l,r-1,i}.$$

Proof. Let $\bullet \in \{\varnothing, \star\}$. From the same argument in [SW1, Lemma 2.1, Proposition 2.2], we see that the sum of the product

$$\sum_{(k_1,\dots,k_{r-1},l)\in I_{k,r,i}} \zeta_{\mathcal{F}_2}(l)\zeta^{\bullet}_{\mathcal{F}_2}(k_1,\dots,k_{r-1}) = \sum_{l=1}^{k-r} \zeta_{\mathcal{F}_2}(l) S^{\bullet}_{\mathcal{F}_2;k-l,r-1,i}$$

coincides with the left-hand side of the desired recurrence relation by the harmonic relation for $\mathcal{F}_2$-MZVs. □

COROLLARY 5.6. *If k is even, then we have*

$$(r-i)S_{\mathcal{F}_2;k,r,i} + iS_{\mathcal{F}_2;k,r,i+1} + (k-r)S_{\mathcal{F}_2;k,r-1,i} = 0,$$
$$(r-i)S^{\star}_{\mathcal{F}_2;k,r,i} + iS^{\star}_{\mathcal{F}_2;k,r,i+1} - (k-r)S^{\star}_{\mathcal{F}_2;k,r-1,i} = 0$$

for positive integers k, r, i with $2 \le i+1 \le r \le k-1$.

Proof. If l is odd, then $\zeta_{\mathcal{F}_2}(l) = 0$ by Theorem 3.2 or (3.8). If l is even, then $\zeta_{\mathcal{F}_2}(l)$ is a multiple of $x_{\mathcal{F}}$ by Theorem 3.2 or (3.8) and $S^{\bullet}_{\mathcal{F}_2;k-l,r-1,i}$ is also a multiple of $x_{\mathcal{F}}$ by Saito–Wakabayashi and Murahara's sum formulas. □

Proof of Theorem 5.4. We prove the non-star case by backward induction on $r \le k-1$. Since

$$\begin{aligned} b_{k,k-1,i} &= \binom{k-1}{k-1} + (-1)^{k-1-i}\left\{(k-k+1)\binom{k}{i-1} + \binom{k-1}{i-1} + (-1)^{k-2}\binom{k-1}{k-1-i}\right\} \\ &= 1 + (-1)^{i-1}\binom{k+1}{i}, \end{aligned}$$

we have

$$\begin{aligned} S_{\mathcal{F}_2;k,k-1,i} &= \zeta_{\mathcal{F}_2}(\{1\}^{i-1}, 2, \{1\}^{k-i-1}) = \frac{1}{2}\left\{1 + (-1)^{i-1}\binom{k+1}{i}\right\} \mathfrak{Z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2} \\ &= \frac{b_{k,k-1,i}}{2} \cdot \mathfrak{Z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2}, \end{aligned}$$

by the definition of $S_{\mathcal{F}_2;k,r,i}$ and (3.24). Hence, the case $r = k-1$ is true. To complete the induction step, by Corollary 5.6, it suffices to prove that

$$(r-i)b_{k,r,i} + ib_{k,r,i+1} - (k-r)b_{k,r-1,i} = 0 \tag{5.7}$$

holds for $2 \le r \le k-1$. The left-hand side of (5.7) is

$$\begin{aligned} &(r-i)\left[\binom{k-1}{r} + (-1)^{r-i}\left\{(k-r)\binom{k}{i-1} + \binom{k-1}{i-1} + (-1)^{r-1}\binom{k-1}{r-i}\right\}\right] \\ &\quad +i\left[\binom{k-1}{r} + (-1)^{r-i-1}\left\{(k-r)\binom{k}{i} + \binom{k-1}{i} + (-1)^{r-1}\binom{k-1}{r-i-1}\right\}\right] \\ &-(k-r)\left[\binom{k-1}{r-1} + (-1)^{r-i-1}\left\{(k-r+1)\binom{k}{i-1} + \binom{k-1}{i-1} + (-1)^{r-2}\binom{k-1}{r-i-1}\right\}\right] \end{aligned}$$

by definition. By $\binom{k-1}{r-1} = \frac{r}{k-r}\binom{k-1}{r}$, we have

$$(r-i)\binom{k-1}{r} + i\binom{k-1}{r} - (k-r)\binom{k-1}{r-1} = 0. \tag{5.8}$$

By $\binom{k}{i} = \frac{k-i+1}{i}\binom{k}{i-1}$, we have

$$(r-i)(k-r)\binom{k}{i-1} - i(k-r)\binom{k}{i} + (k-r)(k-r+1)\binom{k}{i-1} = 0. \tag{5.9}$$

By $\binom{k-1}{i} = \frac{k-i}{i}\binom{k-1}{i-1}$, we have

$$(r-i)\binom{k-1}{i-1} - i\binom{k-1}{i} + (k-r)\binom{k-1}{i-1} = 0. \tag{5.10}$$

By $\binom{k-1}{r-i} = \frac{k-r+i}{r-i}\binom{k-1}{r-i-1}$, we have

$$(r-i)\binom{k-1}{r-i} - i\binom{k-1}{r-i-1} - (k-r)\binom{k-1}{r-i-1} = 0. \tag{5.11}$$

From (5.8), (5.9), (5.10) and (5.11), we obtain (5.7) and we complete the proof of the formula for $S_{\mathcal{F}_2;k,r,i}$. In the star case, we should prove

$$S^{\star}_{\mathcal{F}_2;k,k-1,i} = \frac{b^{\star}_{k,k-1,i}}{2} \cdot \mathfrak{Z}_{\mathcal{F}_2}(k+1)x_{\mathcal{F}_2}$$

and the recurrence relation

$$(r-i)b^{\star}_{k,r,i} + ib^{\star}_{k,r,i+1} - (k-r)b^{\star}_{k,r-1,i} = 0.$$

These are proved similarly to the non-star case. □

REMARK 5.7. We can also prove the star case by connecting $S_{\mathcal{F}_2;k,r,i}$ and $S^{\star}_{\mathcal{F}_2;k,r,i}$ directly using Proposition 2.5. This is the method used in [SY].

Appendix

A. Proof of equality (3.26)

In this appendix, we prove the following proposition.

PROPOSITION A.1. *For non-negative integers a and b, we have*

$$C = 1 + (-1)^a \binom{a+b+3}{b+2};$$

see the proof of Theorem 3.13 for the definition of C.

We divide C into six parts. Set

$$\mathrm{I} := (-1)^{a+1} \sum_{\substack{l+m=b-1 \\ l,m\geq 0}} \sum_{\substack{r+s=a \\ r,s\geq 0}} (-1)^{s+m} \binom{r+l+1}{r}\binom{s+m+1}{s}\binom{a+b+3}{s+m+2},$$

$$\mathrm{II} := (-1)^{a+1} \sum_{\substack{l+m=b-1 \\ l,m\geq 0}} \sum_{\substack{r+s=a \\ r,s\geq 0}} \binom{r+l+1}{r}\binom{s+m+1}{s},$$

$$\mathrm{III} := 2(-1)^a \sum_{\substack{r+s=a \\ r,s\geq 0}} (-1)^s \binom{r+b+1}{r}\binom{a+b+3}{s+1},$$

$$\mathrm{IV} := 2(-1)^{a+1} \sum_{\substack{r+s=a \\ r,s\geq 0}} \binom{r+b+1}{r},$$

$$\mathrm{V} := \sum_{\substack{m+n=a-1 \\ m,n\geq 0}} (-1)^n \sum_{\substack{r+s=n \\ r,s\geq 0}} (-1)^{s+m+1} \binom{r+b+1}{r}\binom{s+m+1}{s}\binom{a+b+3}{s+m+2},$$

$$\mathrm{VI} := \sum_{\substack{m+n=a-1 \\ m,n\geq 0}} (-1)^{n+1} \sum_{\substack{r+s=n \\ r,s\geq 0}} \binom{r+b+1}{r}\binom{s+m+1}{s}.$$

Note that we easily obtain

$$\mathrm{IV} = 2(-1)^{a+1}\binom{a+b+2}{a}. \tag{A.1}$$

By the definition of negative binomial coefficients and the Chu–Vandermonde identity, we also have

$$\mathrm{II} = (-1)^{a+1} b \binom{a+b+2}{a}, \qquad \mathrm{VI} = (-1)^a \binom{a+b+1}{a-1}. \tag{A.2}$$

Next, we calculate I, III and V. We use the following equality repeatedly:

$$\sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{1}{x+k} = \frac{n!}{x(x+1)\cdots(x+n)}. \tag{A.3}$$

Here, n is a non-negative integer and x is an indeterminate.

LEMMA A.2.

$$I = 0.$$

Proof. By elementary calculations, we have

$$\begin{aligned}
\mathrm{I} &= (-1)^{a+1}\sum_{m=0}^{b-1}\sum_{s=0}^{a}(-1)^{s+m}\binom{a+b-m-s}{b-m}\binom{s+m+1}{s}\binom{a+b+3}{s+m+2}\\
&= (-1)^{a+1}(a+1)\binom{a+b+2}{a+1}\sum_{s=0}^{a}(-1)^s\binom{a}{s} \qquad \text{(A.4)}\\
&\quad\times\sum_{m=0}^{b-1}(-1)^m\binom{b+1}{m+1}\left(\frac{1}{a+b+1-s-m}+\frac{1}{s+m+2}\right).
\end{aligned}$$

Applying (A.3) with $x = -(a+b+2-s)$ and $x = s+1$, we have

$$\begin{aligned}
&\sum_{m=0}^{b-1}(-1)^m\binom{b+1}{m+1}\left(\frac{1}{a+b+1-s-m}+\frac{1}{s+m+2}\right)\\
&= \sum_{m=0}^{b+1}(-1)^{m-1}\binom{b+1}{m}\left(\frac{1}{a+b+2-s-m}+\frac{1}{s+m+1}\right)\\
&\quad+\left(\frac{1}{a+b+2-s}+\frac{1}{s+1}\right)+(-1)^{b+1}\left(\frac{1}{a+1-s}+\frac{1}{s+b+2}\right) \qquad \text{(A.5)}\\
&= \frac{(-1)^b}{a+b+2-s}\binom{a+b+1-s}{b+1}^{-1}-\frac{1}{s+1}\binom{b+s+2}{b+1}^{-1}\\
&\quad+\frac{1}{a+b+2-s}+\frac{1}{s+1}+\frac{(-1)^{b+1}}{a+1-s}+\frac{(-1)^{b+1}}{s+b+2}.
\end{aligned}$$

By substituting (A.5) into (A.4) and then using (A.3) again, we have

$$(-1)^{a+b+1}\sum_{s=0}^{a}(-1)^s\binom{a+b+2}{s} = (-1)^{b+1}\binom{a+b+1}{a},$$

$$(-1)^{a}\sum_{s=0}^{a}(-1)^s\binom{a+b+2}{a-s} = \sum_{s=0}^{a}(-1)^s\binom{a+b+2}{s} = (-1)^{a}\binom{a+b+1}{a},$$

$$(-1)^{a+1}(a+1)\binom{a+b+2}{a+1}\sum_{s=0}^{a}(-1)^s\binom{a}{s}\frac{1}{a+b+2-s} = -1,$$

$$(-1)^{a+1}(a+1)\binom{a+b+2}{a+1}\sum_{s=0}^{a}(-1)^s\binom{a}{s}\frac{1}{s+1} = (-1)^{a+1}\binom{a+b+2}{a+1},$$

$$(-1)^{a+b}(a+1)\binom{a+b+2}{a+1}\sum_{s=0}^{a}(-1)^s\binom{a}{s}\frac{1}{a+1-s} = (-1)^{b}\binom{a+b+2}{a+1},$$

$$(-1)^{a+b}(a+1)\binom{a+b+2}{a+1}\sum_{s=0}^{a}(-1)^s\binom{a}{s}\frac{1}{s+b+2}=(-1)^{a+b}.$$

Since $a+b$ is even, we have the conclusion. □

LEMMA A.3.

$$\mathrm{III}=2+2(-1)^a\binom{a+b+2}{a+1}.$$

Proof. By (A.3), we have

$$\begin{aligned}
\mathrm{III}&=2(-1)^a\sum_{s=0}^{a}(-1)^s\binom{a+b+1-s}{a-s}\binom{a+b+3}{s+1}\\
&=2(-1)^{a-1}(a+b+3)\binom{a+b+2}{a+1}\left\{\sum_{s=0}^{a+1}(-1)^s\binom{a+1}{s}\frac{1}{a+b+3-s}-\frac{1}{a+b+3}\right\}\\
&=2(-1)^{a-1}(a+b+3)\binom{a+b+2}{a+1}\left\{\frac{(-1)^{a-1}}{a+b+3}\binom{a+b+2}{a+1}^{-1}-\frac{1}{a+b+3}\right\}\\
&=2+2(-1)^a\binom{a+b+2}{a+1},
\end{aligned}$$

which completes the proof. □

LEMMA A.4.

$$V=(-1)^a a\binom{a+b+2}{a+1}+(-1)^a\binom{a+b+1}{a}-1.$$

Proof. Since

$$\begin{aligned}
\mathrm{V}&=(-1)^a\sum_{n=0}^{a-1}\sum_{s=0}^{n}(-1)^s\binom{b+n+1-s}{b+1}\binom{a+s-n}{s}\binom{a+b+3}{a+s+1-n}\\
&=(-1)^a(a+1)\binom{a+b+2}{a+1}\sum_{n=0}^{a-1}\binom{a}{n}\\
&\qquad\times\sum_{s=0}^{n}(-1)^s\binom{n}{s}\left(\frac{1}{a+s+1-n}+\frac{1}{b+2+n-s}\right)
\end{aligned}$$

and

$$\begin{aligned}
\sum_{s=0}^{n}(-1)^s\binom{n}{s}\frac{1}{a+s+1-n}&=\frac{1}{a+1-n}\binom{a+1}{n}^{-1},\\
\sum_{s=0}^{n}(-1)^s\binom{n}{s}\frac{1}{b+2+n-s}&=\frac{(-1)^n}{b+2+n}\binom{b+n+1}{b+1}^{-1}
\end{aligned}$$

hold by (A.3), we obtain the desired formula. □

Proof of Proposition 3.26. From (A.1), (A.2), Lemmas A.2, A.3, and A.4, we obtain the desired formula. □

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Masataka ONO
Global Education Center, Waseda University
1–6–1 Nishi-Waseda,
Shinjuku-ku, Tokyo 169–8050
Japan
e-mail: m-ono@aoni.waseda.jp

Kosuke SAKURADA
Seiwa Gakuen High School
3–4–1, Kinoshita, Wakabayashi-ku,
Sendai 984–0047
Japan
e-mail: sakurada.kosuke@seiwa.ac.jp

Shin-ichiro SEKI
Department of Mathematical Sciences
Aoyama Gakuin University
5–10–1 Fuchinobe, Chuo-ku, Sagamihara-shi,
Kanagawa 252–5258
Japan
e-mail: seki@math.aoyama.ac.jp