SUPERCONGRUENCES OF MULTIPLE HARMONIC $q$-SUMS AND GENERALIZED FINITE/SYMMETRIC MULTIPLE ZETA VALUES

YOSHIHIRO TAKEYAMA AND KOJI TASAKA

Abstract. The Kaneko–Zagier conjecture describes a correspondence between finite multiple zeta values and symmetric multiple zeta values. Its refined version has been established by Jarossay, Rosen and Ono–Seki–Yamamoto. In this paper, we explicate these conjectures through studies of multiple harmonic $q$-sums. We show that the (generalized) finite/symmetric multiple zeta value are obtained by taking an algebraic/analytic limit of multiple harmonic $q$-sums. As applications, new proofs of reversal, duality and cyclic sum formulas for the generalized finite/symmetric multiple zeta values are given.

1. Introduction

In 2013, Kaneko and Zagier [KZ] posed a conjecture (called the Kaneko–Zagier conjecture) about a correspondence between the finite multiple zeta value $\zeta_A(k) \in A = (\prod_p \mathbb{Z}/p\mathbb{Z})/(\bigoplus_p \mathbb{Z}/p\mathbb{Z})$, where $p$ runs over all primes, and the symmetric multiple zeta value $\zeta_S(k) \in \mathbb{Z}/\pi^2\mathbb{Z}$, where $\mathbb{Z}$ denotes the $\mathbb{Q}$-vector space spanned by all multiple zeta values. Recently, its refined version has been established by Jarossay [Jar2, Conjecture 5.3.2], Rosen [Ros19, Conjecture 2.3] and Ono–Seki–Yamamoto [OSY21, Conjecture 4.3]. In this paper, we explicate these conjectures through studies of multiple harmonic $q$-sums.

In [BTT18], the authors developed a new approach to simultaneously give relations among both $\zeta_A(k)$’s and $\zeta_S(k)$’s over $\mathbb{Q}$, and partially support the Kaneko–Zagier conjecture. An epoch-making invention is that both $\zeta_A(k)$ and $\zeta_S(k)$ are obtained from certain limiting values of a multiple harmonic $q$-sum $H_{p-1}(k; q)$ (defined in (2.6)) at $q$ being primitive $p$-th roots of unity. In the current paper, this result is recast by introducing a $\mathbb{Q}$-multiple zeta value $\zeta_Q(k)$ made from the sequence $(H_{p-1}(k; q) \mod [p])_p$, where $[p] = (1 - q^p)/(1 - q)$ and $p$ runs over all prime numbers.
primes. Constructing two algebra maps $\phi_A$ and $\phi_S$, we prove in Theorem 2.8 that
\begin{equation}
\phi_A(\zeta_{\mathcal{Q}}(k)) = \zeta_A(k) \quad \text{and} \quad \phi_S(\zeta_{\mathcal{Q}}(k)) \equiv \zeta_S(k) \mod \pi i \mathbb{Z}[\pi i].
\end{equation}
As an application, from a family of relations among $\zeta_{\mathcal{Q}}(k)$’s, one obtains the corresponding family of relations among both $\zeta_A(k)$’s and $\zeta_S(k)$’s in the same form. These results, together with the statement of the Kaneko–Zagier conjecture, are summarized in §2.

In §3, we explicate a refined version of the Kaneko–Zagier conjecture, which is initiated by Hirose, Rosen and Jarossay, independently. It describes a conjectural relationship between the $\mathcal{A}$-multiple zeta value $\zeta_{\mathcal{A}}(k)$ and the $\mathcal{S}$-multiple zeta value $\zeta_{\mathcal{S}}(k)$, lying in the $\mathbb{Q}$-algebras $\mathcal{A}$ and $\mathcal{S}$, respectively. Although there are natural surjections $\mathcal{A} \to \mathcal{A}$ and $\mathcal{S} \to \mathcal{S}$, which send $\zeta_{\mathcal{A}}(k) \mapsto \zeta_{\mathcal{A}}(k)$ and $\zeta_{\mathcal{S}}(k) \mapsto \zeta_{\mathcal{S}}(k)$, respectively, the relationship between the Kaneko–Zagier conjecture and its refined version is not clearly written in the literature. For future reference, we prove in Proposition 3.6 that the refined version implies the Kaneko–Zagier conjecture under the assumption that Rosen’s lifting conjecture holds.

Our new story starts from §4, where we introduce a “$q$-analogue” $\mathcal{Q}$ of the $\mathbb{Q}$-algebra $\mathcal{A}$. In the $\mathbb{Q}$-algebra $\mathcal{Q}$, for each index $k$ we define a unified object $\zeta_{\mathcal{Q}}(k)$, called the $\mathcal{Q}$-multiple zeta value (Definition 4.2). As a generalization of (1.1), we show in Theorems 4.3 and 4.4 that
\begin{equation}
\phi_{\mathcal{A}}(\zeta_{\mathcal{Q}}(k)) = \zeta_{\mathcal{A}}(k) \quad \text{and} \quad \phi_{\mathcal{S}}(\zeta_{\mathcal{Q}}(k)) = \zeta_{\mathcal{S}}(k) \mod \pi i,
\end{equation}
which are our main results of this paper. We will also compute images of other variants (a star version and a ‘conjugate model’) of multiple harmonic $q$-sums under the maps $\phi_{\mathcal{A}}$ and $\phi_{\mathcal{S}}$. Applying these results to relations among $\mathcal{Q}$-multiple zeta values, we obtain relations among both $\zeta_{\mathcal{A}}(k)$’s and $\zeta_{\mathcal{S}}(k)$’s in the same form, which also support the refined version of the Kaneko–Zagier conjecture.

As examples of relations, we extend the reversal, duality and cyclic sum formulas for both the $\mathcal{A}$-multiple zeta value and the $\mathcal{S}$-multiple zeta value obtained in [HMO, Jar2, Kaw19, OSY21, Ros15, Sek19] to corresponding formulas for $\mathcal{Q}$-multiple zeta values. This will be the subject in §5.

§6 is devoted to computing dimensions of the $\mathbb{Q}$-vectors space spanned by $\mathbb{Q}$-multiple zeta values, based on experimental works. We indicate that all $\mathbb{Q}$-linear relations among $\mathcal{F}$-multiple zeta values ($\mathcal{F} \in \{A, S\}$) of weight up to 5 may be obtained from relations among variants of $\mathcal{Q}$-multiple zeta values. We also study relations of $\zeta_{\mathcal{Q}}(k) = (H_{p-1}(k; q) \mod [p]^2)_p$. 
Notation. In this paper, we often use the following notation. We call a finite ordered list \( \mathbf{k} = (k_1, \ldots, k_d) \) of positive integers an index and write \( \text{wt}(\mathbf{k}) = k_1 + \cdots + k_d \) (weight) and \( \text{dep}(\mathbf{k}) = d \) (depth). An index \( \mathbf{k} = (k_1, \ldots, k_d) \) is called admissible if \( k_1 \geq 2 \). We allow the empty index \( \emptyset \) to be the unique index \( \mathbf{k} \) such that \( \text{wt}(\mathbf{k}) = \text{dep}(\mathbf{k}) = 0 \). For any function \( F \) on indices, set \( F(\emptyset) = 1 \). For tuples \( \mathbf{k} = (k_1, \ldots, k_d) \) and \( \mathbf{l} = (l_1, \ldots, l_d) \), we write \( (\mathbf{k} + \mathbf{l}) = (k_1 + l_1, \ldots, k_d + l_d) \), \( b\left(\begin{array}{c} k \\ l \end{array}\right) := \prod_{j=1}^{d} \frac{k_j + l_j - 1}{l_j} \), \( \overline{\mathbf{k}} := (k_d, \ldots, k_1) \), \( \mathbf{k}_a := (k_1, \ldots, k_a) \), \( \mathbf{k}^a := (k_{a+1}, \ldots, k_d) \) \((0 \leq a \leq d)\), where \( \mathbf{k}_0 = \mathbf{k}^d = \emptyset \).

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2. Kaneko–Zagier conjecture and its \( q \)-analogue view points

In this section, we first recall the Kaneko–Zagier conjecture on a correspondence between finite multiple zeta values (\( A \)-MZVs) and symmetric multiple zeta values (\( S \)-MZVs). Then, we recast the work of [BTT18].

2.1. MZV. The multiple zeta value (abbreviated by MZV) is defined for an admissible index \( \mathbf{k} = (k_1, \ldots, k_d) \) by

\[
\zeta(\mathbf{k}) = \sum_{m_1 > \cdots > m_d > 0} \frac{1}{m_1^{k_1} \cdots m_d^{k_d}} \in \mathbb{R}.
\]

Let \( \mathcal{Z}_k \) denote the \( \mathbb{Q} \)-vector space spanned by all MZVs of weight \( k \). The sum

\[
\mathcal{Z} = \sum_{k \geq 0} \mathcal{Z}_k
\]

forms a \( \mathbb{Q} \)-algebra. Zagier [Zag94] observed that the equality \( \dim_{\mathbb{Q}} \mathcal{Z}_k = d_k \) holds for all \( k \geq 0 \), where \( d_k \) is given by \( \sum_{k \geq 0} d_k x^k = 1/(1 - x^2 - x^3) \). Goncharov [Gon01] and Terasoma [Ter02] showed independently the inequality \( \dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k \) for all \( k \). This observation/result tells us that MZVs satisfy numerous linear relations over \( \mathbb{Q} \). The first example of relations is \( \zeta(3) = \zeta(2, 1) \), which was discovered by Euler [Eul76]. Since 1990’s, explicit families of relations, such as the sum formula [Gra97], the cyclic sum formula [HO03], the duality formula [Zag94], the regularized double
shuffle relation [IKZ06, Rac02] and so on, have been intensively studied by various approaches and also applied in several branches of mathematics and physics.

**Regularizations.** As a basic of MZVs, we quickly recall the shuffle and the stuffle regularization of MZVs, mainly following [IKZ06, §2].

Let \( h = \mathbb{Q}\langle x_0, x_1 \rangle \) be the non-commutative polynomial algebra over \( \mathbb{Q} \) and set \( h^1 = \mathbb{Q} + h x_1 \). Define the shuffle product \( \shuffle : h \otimes h \to h \) inductively by

\[
uw \shuffle vw' = u(w \shuffle vw') + v(uw \shuffle w')
\]

for \( w, w' \in h \) and \( u, v \in \{x_0, x_1\} \), with the initial condition \( w \shuffle 1 = w = 1 \shuffle w \). Equipped with the shuffle product, the vector space \( h \) forms a commutative \( \mathbb{Q} \)-algebra and \( h^1 \) is its \( \mathbb{Q} \)-subalgebra. We write \( h/\mathbb{A}_1 \) and \( h^1/\mathbb{A}_1 \) for the commutative \( \mathbb{Q} \)-algebras with the shuffle product. It is known that \( h/\mathbb{A}_1 \cong h^1/\mathbb{A}_1[x_0] \). For an index \( k = (k_1, \ldots, k_d) \) we write

\[
x_k = x_0^{k_1-1} x_1 \cdots x_0^{k_d-1} x_1,
\]

which forms a \( \mathbb{Q} \)-linear basis of \( h^1 \).

Let \( \mathfrak{h}^1 = \mathbb{Q}\langle y_k \mid k \geq 1 \rangle \) be the non-commutative polynomial algebra over \( \mathbb{Q} \). Define the stuffle product \( \ast : \mathfrak{h}^1 \otimes \mathfrak{h}^1 \to \mathfrak{h}^1 \) inductively by

\[
y_kw \ast y_lw' = y_k(w \ast y_lw') + y_l(y_kw \ast w') + y_{k+l}(w \ast w')
\]

for \( w, w' \in \mathfrak{h}^1 \) and \( k, l \geq 1 \), with the initial condition \( w \ast 1 = w = 1 \ast w \). Equipped with the stuffle product, the vector space \( \mathfrak{h}^1 \) forms a commutative \( \mathbb{Q} \)-algebra and we denote it by \( \mathfrak{h}^1_\ast \). For an index \( k = (k_1, \ldots, k_d) \) we also write

\[
y_k = y_{k_1} \cdots y_{k_d},
\]

which forms a \( \mathbb{Q} \)-linear basis of \( \mathfrak{h}^1 \). Since we use Racinet’s formulation of the regularization theorem later (see (A.17)), we distinguish \( \mathfrak{h}^1 \) (y-words) from \( h^1 \) (x-words), while the \( \mathbb{Q} \)-linear map \( \mathfrak{h}^1 \to h^1 \), \( y_k \mapsto x_k \) is an isomorphism of \( \mathbb{Q} \)-vector spaces.

There are algebra homomorphisms

\[
Z^\shuffle : h^1_\shuffle \to \mathbb{R}[T] \quad \text{and} \quad Z^* : \mathfrak{h}^1_\ast \to \mathbb{R}[T]
\]

such that \( Z^\shuffle(x_1) = T \), \( Z^*(y_1) = T \) and

\[
Z^\shuffle(x_k) = Z^*(y_k) = \zeta(k)
\]

for all admissible index \( k \) (see [IKZ06, Proposition 1]). For an index \( k \) we write

\[
(2.1) \quad \zeta^\shuffle(k; T) = Z^\shuffle(x_k) \quad \text{and} \quad \zeta^*(k; T) = Z^*(y_k),
\]

which are called the shuffle and the stuffle regularized MZV, respectively. These are elements in the polynomial ring \( \mathbb{Z}[T] \) over the \( \mathbb{Q} \)-algebra \( \mathbb{Z} \).
2.2. Multiple harmonic sum modulo \( p \). For a positive integer \( m \) and an index \( k = (k_1, \ldots, k_d) \), we define the multiple harmonic sum \( H_m(k) \in \mathbb{Q} \) by
\[
H_m(k) = H_m(k_1, \ldots, k_d) = \sum_{m_1 > \cdots > m_d > 0} \frac{1}{m_1^{k_1} \cdots m_d^{k_d}}.
\]
We understand \( H_m(k) = 0 \) if \( \text{dep}(k) > m \). Zhao [Zha08] and Hoffman [Hof15] independently discovered mod \( p \) congruence relations among \( H_{p-1}(k) \)'s, which holds for all large primes \( p \). A prototypical example is Hoffman’s duality ([Hof15, Theorem 4.6]); for each index \( k \) and all primes \( p \), it holds that
\[
(2.2) \quad H_{p-1}^\star(k) + H_{p-1}^\star(k^\vee) \equiv 0 \mod p,
\]
where we set
\[
H_{m}^\star(k_1, \ldots, k_d) = \sum_{m_1 \geq \cdots \geq m_d > 0} \frac{1}{m_1^{k_1} \cdots m_d^{k_d}}
\]
and the index \( k^\vee \) is called Hoffman’s dual index obtained by writing each component \( k_i \) as a sum of 1 and then interchanging commas ‘,‘ and plus signs ‘+’. For example,
\[
(3, 1)^\vee = (1 + 1 + 1, 1)^\vee = (1, 1, 1 + 1) = (1, 1, 2).
\]

2.3. \( \mathcal{A} \)-MZV. A study of finite multiple zeta values has been initiated by Kaneko–Zagier [KZ]. A crucial feature is that mod \( p \) congruence relations among \( H_{p-1}(k) \)'s being independent from choices of large primes \( p \), such as (2.2), turn out to be \( \mathbb{Q} \)-linear relations among finite multiple zeta values, which we now define in the ring
\[
\mathcal{A} = \left( \prod_{p \text{ prime}} \mathbb{Z}/p\mathbb{Z} \right) / \left( \bigoplus_{p \text{ prime}} \mathbb{Z}/p\mathbb{Z} \right).
\]

The above ring \( \mathcal{A} \) is due to Kontsevich [Kon09, §2.2] and its ring structure is given by the component-wise addition and multiplication. We denote by \( (a_p)_p \) an element in \( \mathcal{A} \), where \( p \) runs over all primes and \( a_p \in \mathbb{Z}/p\mathbb{Z} \). An element \( (a_p)_p \) in \( \mathcal{A} \) equals the zero element \( 0 \in \mathcal{A} \), if and only if \( a_p = 0 \) for all large enough \( p \). For simplicity of notation, we will view \( (c_p \mod p)_p \) as an element in \( \mathcal{A} \) for each sequence \( \{c_a\}_{a \geq 0} \subset \mathbb{Q} \) such that the denominator of \( c_p \) may be divisible by \( p \) for finitely many primes \( p \) (to be precise, for such \( p \) we should replace \( c_p \) with any elements in \( \mathbb{Z}/p\mathbb{Z} \)). Under this notation, the map \( \mathbb{Q} \to \mathcal{A}, c \mapsto (c \mod p)_p \) is well-defined and it induces scalar multiplication of \( \mathbb{Q} \) on \( \mathcal{A} \). Thus, \( \mathcal{A} \) forms a \( \mathbb{Q} \)-algebra.

**Definition 2.1.** The finite multiple zeta value (call it \( \mathcal{A} \)-MZV for short) is defined for each index \( k \) by
\[
\zeta_{\mathcal{A}}(k) = (H_{p-1}(k) \mod p)_p \in \mathcal{A}.
\]
Its star version (called \( \mathcal{A} \)-MZSV) is denoted by \( \zeta_{\mathcal{A}}^\star(k) \), replacing \( H_{p-1}(k) \) with \( H_{p-1}^\star(k) \).
Let $\mathcal{Z}_k^A$ be the $\mathbb{Q}$-vector subspace of $A$ spanned by all $A$-MZVs of weight $k$. Set

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

It follows that the $\mathbb{Q}$-linear map $\delta_1^A: \mathcal{Z}_k^A \to \mathcal{Z}_k^A$, $y_k \mapsto \zeta_A(k)$ forms a $\mathbb{Q}$-algebra map. Zagier numerically observed that $\dim_{\mathbb{Q}} \mathcal{Z}_k^A \approx d_k - d_{k-2}$ for $k \geq 2$. Hence, $A$-MZVs also satisfy many relations over $\mathbb{Q}$. As an example of relations, since (2.2) holds for all sufficiently large primes, we obtain

$$\zeta_A^\star(k) + \zeta_A(\kappa^\vee) = 0.$$  

The above relation (2.3) is called Hoffman’s duality for the $A$-MZSV.

### 2.4. $S$-MZV

With a hint by Kontsevich (see [Kan19, §9]), Kaneko–Zagier introduced a real counter part of $A$-MZVs. Recall the notation (1.3) and the regularized MZV (2.1). For an index $k$ and $\bullet \in \{\ast, \sqcup\}$, we define

$$\zeta_{S}^\bullet(k) = \sum_{a=0}^{\text{dep}(k)} (-1)^{\omega(k_a)} \zeta^\bullet(k_a; T) \zeta^\bullet(k^\ast; T).$$

It is shown in [KZ] (see also [Kan19]) that the right side does not depend on $T$ and that

$$\zeta_{S}^\ast(k) \equiv \zeta_{S}^\sqcup(k) \mod \pi^2 \mathcal{Z}$$

holds for any index $k$. The following definition is therefore independent of the choice of regularizations.

**Definition 2.2.** For each index $k$, we define the symmetric multiple zeta value $\zeta_{S}(k)$ (call it $S$-MZV for short) by

$$\zeta_{S}(k) = \zeta_{S}^\ast(k) \mod \pi^2 \mathcal{Z}.$$  

Its star version ($S$-MZSV) is defined by

$$\zeta_{S}^\star(k_1, \ldots, k_d) = \sum_{\square \text{ is either a comma },{,}' \text{ or a plus }'+'} \zeta_{S}(k_1\square \cdots \square k_d).$$

Note that the above expression of $S$-MZSV naturally arises from the standard decomposition of $H_{m}^\ast(k)$ in terms of $H_m(k)$. For example, we have

$$H_{m}^\ast(k_1, k_2) = \sum_{m \geq m_1 \geq m_2 \geq 1} \frac{1}{m_{1}^{k_{1}} m_{2}^{k_{2}}} = \left( \sum_{m \geq m_1 \geq m_2 \geq 1} \sum_{m \geq m_1 = m_2 \geq 1} \right) \frac{1}{m_{1}^{k_{1}} m_{2}^{k_{2}}}$$

$$= H_m(k_1, k_2) + H_m(k_1 + k_2),$$

which corresponds to the definition $\zeta_{S}^\ast(k_1, k_2) = \zeta_{S}(k_1, k_2) + \zeta_{S}(k_1 + k_2)$. 
By definition, $S$-MZV is a $\mathbb{Q}$-linear combination of MZVs modulo $\pi^2 \mathbb{Z}$. The opposite statement, namely, the $\mathbb{Q}$-vector space $\overline{\mathbb{Z}} = \mathbb{Z}/\pi^2 \mathbb{Z}$ is generated by $S$-MZVs, was shown by Yasuda [Yas16].

2.5. $A$-MZV vs. $S$-MZV. This paper deals with the following variant of the Kaneko–Zagier conjecture [KZ].

**Conjecture 2.3.** Let $k$ be a positive integer. For rational numbers $c_k$ we have

$$\sum_{\text{wt}(k) = k} c_k \zeta_A(k) = 0 \iff \sum_{\text{wt}(k) = k} c_k \zeta_S(k) = 0,$$

where the sum $\sum_{\text{wt}(k) = k}$ runs over all indices $k$ of weight $k$.

Conjecture 2.3 implies that the $\mathbb{Q}$-linear map sending $\zeta_A(k)$ to $\zeta_S(k)$ for each index $k$ of weight $k$ is an isomorphism from $\mathbb{Z}_k^A$ to $\mathbb{Z}_k^A / \pi^2 \mathbb{Z}_{k-2}$. As evidences, several families of relations which are satisfied by both $A$-MZVs and $S$-MZVs in the same shape are known. For one, as a counterpart of (2.3), the relation

$$\zeta_S^*(k) + \zeta_S^*(k^\vee) = 0$$

holds for any index $k$.

Note that (2.4) is equivalent to the statement for the star version, because by inclusion-exclusion, for $\mathcal{F} \in \{A, S\}$ we have

$$\zeta_\mathcal{F}(k_1, \ldots, k_d) = \sum_{\square \text{ is either a comma } ',$$ \text{ or a plus '}+\text{'} } (-1)^{\sharp\{\square = +\}} \zeta_\mathcal{F}^*(k_1 \square \ldots \square k_d).$$

2.6. **Multiple harmonic $q$-sum.** A *multiple harmonic $q$-sum* is defined for a positive integer $m$ and an index $k = (k_1, \ldots, k_d)$ by

$$H_m(k; q) = H_m(k_1, \ldots, k_d; q) = \sum_{m_1 \geq \ldots \geq m_d > 0} \prod_{a=1}^d \frac{q^{(k_a - 1)m_a}}{[m_a]^{k_a}},$$

where for a positive integer $n$, we denote the $q$-integer by $[n] = [n]_q = (1 - q^n)/(1 - q)$. Similarly, its star version is defined by

$$H_m^*(k; q) = H_m^*(k_1, \ldots, k_d; q) = \sum_{m_1 \geq \ldots \geq m_d > 0} \prod_{a=1}^d \frac{q^{(k_a - 1)m_a}}{[m_a]^{k_a}}.$$

Note that by using

$$\frac{q^{(k_1 - 1)m}}{[m]_{k_1}^{k_1}} \frac{q^{(k_2 - 1)m}}{[m]_{k_2}^{k_2}} = \frac{q^{(k_1 + k_2 - 1)m}}{[m]_{k_1 + k_2}^{k_1 + k_2}} + (1 - q) \frac{q^{(k_1 + k_2 - 2)m}}{[m]_{k_1 + k_2 - 1}^{k_1 + k_2 - 1}},$$
the star $H^*_m(k;q)$ can be written as a $\mathbb{Z}[1-q]$-linear combination of non-star $H_m(k;q)$’s (see also [BTT18, Remark 2.2]).

Replacing numerators with $q^{sma}$ ($s_a \in \mathbb{Z}$) in (2.6), we obtain many other variants of multiple harmonic $q$-sums which may play a role in this study (see §6). In our results, the case $s_a = 1$ ($1 \leq a \leq d$) is necessary and hence treated later (see Definition 4.2). Remark that the model (2.6) is studied by Bradley [Bra05-2, Definition 4] as a $q$-analogue of the multiple harmonic sum $H_m(k)$.

In [BTT18], the authors obtained $\mathcal{A}$-MZVs and $\mathcal{S}$-MZVs as certain limits of values of the above multiple harmonic $q$-sums at $q$ being primitive roots of unity. Here we summarize the results.

**Theorem 2.4.** [BTT18, Theorems 1.1 and 1.2]

(i) For a prime $p$, denote by $\zeta_p$ a primitive $p$-th root of unity. Then, under the identification $\mathbb{Z}[[\zeta_p]]/(1-\zeta_p)\mathbb{Z}[[\zeta_p]] \cong \mathbb{Z}/p\mathbb{Z}$, for each index $k$ and $\bullet \in \{\emptyset, \ast\}$ we have

$$H^*_m(k; \zeta_p) \mod (1-\zeta_p)\mathbb{Z}[[\zeta_p]] = \zeta^*_A(k).$$

(ii) For each index $k = (k_1, \ldots, k_d)$ and $\bullet \in \{\emptyset, \ast\}$, we have

$$\lim_{m \to \infty} H^*_m(k; e^{\frac{2\pi i}{m}}) = \xi^*(k) \equiv \zeta^*_S(k) \mod \pi i\mathbb{Z}[\pi i],$$

where

$$\xi(k) = \sum_{a=0}^{\text{dep}(k)} (-1)^{\text{wt}(k_a)} \zeta^* \left( \frac{k_a}{2}, \frac{\pi i}{2} \right) \zeta^* \left( k^a, -\frac{\pi i}{2} \right)$$

and

$$\xi^*(k) = \sum_{\square \text{ is either a comma '},' or a plus '+'} \xi(k_1\square \cdots \square k_d),$$

which are elements in the polynomial ring $\mathbb{Z}[\pi i]$ over $\mathbb{Z}$.

Let us illustrate an application of Theorem 2.4. Suppose that rational numbers $c_k$ satisfy

(2.8) $\sum_{\text{wt}(k)=k} c_k H_{p-1}(k; \zeta_p) = 0$

for all large primes $p > 0$ and any $\zeta_p$ primitive $p$-th roots of unity. Then by Theorem 2.4, we get $\mathbb{Q}$-linear relations among both $\mathcal{A}$-MZVs and $\mathcal{S}$-MZVs in the same shape:

$$\sum_{\text{wt}(k)=k} c_k \zeta_A(k) = 0 \quad \text{and} \quad \sum_{\text{wt}(k)=k} c_k \zeta_S(k) = 0.$$

As an example of relations of the form (2.8), a kind of duality formula

(2.9) $H^*_{p-1}(k; \zeta_p) + (-1)^{\text{wt}(k)} H^*_{p-1}(k^\vee; \zeta_p) = 0$
is shown in [BTT18, Theorem 1.3]. This leads to
\begin{equation}
(2.10) \quad \zeta^*_\mathcal{F}(k) + (-1)^{\text{wt}(k)} \zeta^*_\mathcal{K}(\mathcal{K}) = 0
\end{equation}
for $\mathcal{F} \in \{A, S\}$, which by combining the reversal relation $\zeta^*_\mathcal{K}(k) = (-1)^{\text{wt}(k)} \zeta^*_\mathcal{K}(\mathcal{K})$ reprove (2.3) and (2.5).

2.7. $\mathbb{Q}$-MZV. Let $p$ be a prime. Since $[p] = \prod_{a=1}^{p-1}(q - e^{2\pi i a/p})$, a polynomial $f(q) \in \mathbb{Z}[q]$ satisfies $f(\zeta_p) = 0$ for any $\zeta_p$ primitive $p$-th roots of unity if and only if $f(q) \equiv 0 \mod [p]$ (a stronger statement can be found in Remark 2.9). Hence, the relation (2.8) can be treated in the following ring
\[
\mathbb{Q} = \left( \prod_{p \text{ prime}} \mathbb{Z}_{(p)}[q]/([p]) \right) / \left( \bigoplus_{p \text{ prime}} \mathbb{Z}_{(p)}[q]/([p]) \right),
\]
where $\mathbb{Z}_{(p)}[q]$ denotes the polynomial ring in $q$ over the ring $\mathbb{Z}_{(p)}$ of rational numbers whose denominators are not divisible by $p$. Here $([p])$ denotes the ideal of $\mathbb{Z}_{(p)}[q]$ generated by the irreducible polynomial $[p]$ over $\mathbb{Z}_{(p)}$. An element of $\mathbb{Q}$ is of the form $(a_p)_p$, where $p$ runs over all primes and $a_p \in \mathbb{Z}_{(p)}[q]/([p])$. Similarly to the convention of $A$, we will also regard $(f_p(q) \mod [p])_p$ as an element in $\mathbb{Q}$ for each sequence \{f_n(q)\}_{n \geq 0} \subset \mathbb{Q}[q]$ such that, for finitely many primes $p$, some of denominators of coefficients of $f_p(q)$ in $q$ may be divisible by $p$. With this, the map $\mathbb{Q}[q] \to \mathbb{Q}, f(q) \mapsto (f(q) \mod [p])_p$ is well-defined. Component-wise addition, multiplication and scalar multiplication by $\mathbb{Q}[q]$ equip $\mathbb{Q}$ with the structure of a $\mathbb{Q}[q]$-algebra.

In this framework, we introduce the following object.

**Definition 2.5.** For each index $k$ and $\bullet \in \{\emptyset, \ast\}$, we define $\zeta^*_\mathbb{Q}(k) \in \mathbb{Q}$ by
\[
\zeta^*_\mathbb{Q}(k) = (H^*_{p-1}(k; q) \mod [p])_p.
\]

Note that for each prime $p$ and positive integer $m$ coprime to $p$, since $\gcd([m], [p]) = 1$, the polynomial $[m]$ is invertible modulo $[p]$, and hence the above definition makes sense.

For each weight $k$, one can observe that elements $\zeta_{\mathbb{Q}}(k)$'s satisfy numerous relations of the form
\begin{equation}
(2.11) \quad \sum_{j=0}^{k} (1 - q)^j \sum_{\text{wt}(k)=k-j} c_{k,j}(p) \zeta_{\mathbb{Q}}(k) = 0
\end{equation}
for some polynomials $c_{k,j}(x) \in \mathbb{Q}[x]$, where $p = (p \mod [p])_p \in \mathbb{Q}$. In other words, the elements $(1 - q)^j \zeta_{\mathbb{Q}}(k)$ of weight $k$ satisfy linear relations over $\mathbb{Q}[p]$, where we set the term $1 - q$ to be of weight 1. For example, as a $q$-analogue of the well-known
congruence $H_{p-1}(1) \equiv 0 \mod p$, we have
\begin{equation}
\zeta_Q(1) - \frac{p-1}{2}(1-q) = 0,
\end{equation}
which is due to Andrews [And99]. One can also find other examples in [HHT17] and [Zha13, Zha16]. Our duality formula (2.9) gives
\[\zeta^*_Q(k) + (-1)^{\text{wt}(k)} \zeta^*_Q(k^\vee) = 0,\]
which by (2.7) is also an example of (2.11).

**Remark 2.6.** In [BTT18, §3], the authors introduce the cyclotomic analogue of finite multiple zeta value, which is slightly different from $\zeta_Q(k)$. In our terminology, the cyclotomic analogue is viewed as $\zeta_Q(k) \mod p$ in the quotient ring $Q/pQ$.

**Remark 2.7.** From the definition, our $\zeta_Q(k)$ may be viewed as a “$q$-analogue” of the finite multiple zeta value $\zeta_A(k)$. However, since both $\zeta_A(k)$ and $\zeta_S(k)$ are obtained as certain realizations of $\zeta_Q(k)$ (see (1.1)), it should have its own name, such as a $Q$-multiple zeta value (abbreviated by $Q$-MZV). In particular, since there are many variants of multiple harmonic $q$-sums, our $\zeta_Q(k)$ would be called the $Q$-MZV of Bradley–Zhao’s model.

### 2.8. From $Q$-MZV to $A$-MZV and $S$-MZV.

We first define two $Q$-algebra maps $\phi_A : Q \to A$ and $\phi_S : \mathcal{O} \to \mathbb{C}$, and then, recast Theorem 2.4 via $Q$-MZVs.

For $\phi_A$, we note that if two polynomials $f(q)$ and $g(q)$ over $\mathbb{Z}_{(p)}$ satisfies $f(q) \equiv g(q) \mod [p]$, then $f(1) \equiv g(1) \mod p$. Therefore, there is the natural projection
\[\mathbb{Z}_{(p)}[q]/([p]) \longrightarrow \mathbb{Z}_{(p)}/p\mathbb{Z}_{(p)} \cong \mathbb{Z}/p\mathbb{Z},\]
that sends $q$ to 1. This induces the surjective $Q$-algebra map
\[\phi_A : Q \longrightarrow A, \quad (f_p(q) \mod [p])_p \longmapsto (f_p(1) \mod p)_p.\]

The $Q$-algebra map $\phi_S$ is defined as the composition of $Q$-algebra maps $\lim$ and $ev$ given as follows. Let $Q(\zeta_p)$ be the $p$th cyclotomic field. Set
\[Q_{\text{an}} = \left( \prod_{p:\text{prime}} Q(\zeta_p) \right) / \left( \bigoplus_{p:\text{prime}} Q(\zeta_p) \right).\]
Since $[p] = \prod_{a=1}^{p-1} (q - e^{2\pi ia/p})$, the map
\[ev : Q \longrightarrow Q_{\text{an}}, \quad (f_p(q) \mod [p])_p \longmapsto (f_p(e^{2\pi i/p}))_p\]
is a well-defined $Q$-algebra map. Consider the $Q$-subalgebra
\[\mathcal{O}_{\text{an}} = \left\{ (z_p)_p \in \prod_{p:\text{prime}} Q(\zeta_p) \mid \lim_{p \to \infty} z_p \text{ converges} \right\}.\]
of \( \prod_{p \text{ prime}} Q(\zeta_p) \) and define
\[
\lim : \mathcal{O}^{an} \to \mathbb{C}, \quad (z_p)_p \mapsto \lim_{p \to \infty} z_p.
\]
which is also a \( \mathbb{Q} \)-algebra map. Its kernel contains the \( \mathbb{Q} \)-subalgebra \( \bigoplus_p \mathbb{Q}(\zeta_p) \). Now let
\[
\mathcal{O} = ev^{-1} \left( \mathcal{O}^{an} / \bigoplus_{p \text{ prime}} \mathbb{Q}(\zeta_p) \right) \subset \mathcal{O}
\]
and define the \( \mathbb{Q} \)-algebra map
\[
\phi_S = \lim \circ ev : \mathcal{O} \to \mathbb{C},
\]
which sends \((f_p(q) \mod [p])_p \to \lim_{p \to \infty} f_p(e^{2\pi i/p})\).

Theorem 2.4 is now restated as follows.

**Theorem 2.8.** For all index \( k \) and \( \bullet \in \{\emptyset, *\} \), we have
\[
\phi_A(\zeta^*_Q(k)) = \zeta^*_A(k)
\]
and
\[
\phi_S(\zeta^*_Q(k)) \equiv \zeta^*_S(k) \mod \pi i \mathbb{Z}[\pi i].
\]

**Proof.** The first equation is immediate from the identity
\[
\phi_A((q^{(k-1)m}[m]^{-k} \mod [p])_p) = (m^{-k} \mod p)_p
\]
for any \( m \in \{1, 2, \ldots, p-1\} \). The second congruence is a consequence of Theorem 2.4 (ii). We complete the proof. \( \square \)

An application to the study of \( \mathcal{A} \)-MZVs and \( \mathcal{S} \)-MZVs is as follows. Applying \( \phi_A \) to (2.11), we obtain
\[
\sum_{\text{wt}(k)=k} c_{k,0}(0) \zeta_A(k) = 0.
\]
On the other hand, since \((1-q)^j c_{k,j}(p) \bigg|_{q=e^{2\pi i/p}} = O(p^{\deg c_{k,j}} - j)\), the image of the left side of (2.11) under the map \( \phi_S \) diverges, if \( \deg c_{k,j} > j \). Thus, under the assumption that \( \deg c_{k,j} \leq j \) for all \( k \) and \( j \), the left side of (2.11) lies in \( \mathcal{O} \) and taking \( \phi_S \) gives
\[
\sum_{\text{wt}(k)=k} c_{k,0}(0) \zeta_S(k) = 0,
\]
because \( \phi_S((1-q)^j c_{k,j}(p)\zeta_Q(k)) \in \mathbb{Q}(\pi i)^j \xi(k) \). This shows that the relation (2.11) among \( \mathbb{Q} \)-MZVs with the above assumption gives rise to relations among both \( \mathcal{A} \)-MZVs and \( \mathcal{S} \)-MZVs in the same shape. As a quick example, by (2.12), we get
\[
\zeta_A(1) = 0 \quad \text{and} \quad \zeta_S(1) = 0.
\]
Remark 2.9. One can show that the map $ev$ is injective. This can be checked as follows. Suppose that a primitive $p$-th root of unity $\zeta_p$ is zero of $f_p(q)$ for all but finitely many primes $p$. By the action of $\text{Gal}(\mathbb{Q}(\zeta_p)/\mathbb{Q})$, we see that $\zeta_p^a$ ($1 \leq a \leq p-1$) is also zero of $f_p(q)$. Hence, $f_p(q)$ is divisible by $[p]$. It is worth mentioning that the injectivity of the map $ev$ implies that the equation (2.11) holds if and only if

$$\sum_{j=0}^{k} (1 - \zeta_p)^j \sum_{\text{wt}(k)=k-j} c_{k,j}(p) H_{p-1}(k; \zeta_p) = 0$$

holds in $\mathbb{Q}(\zeta_p)$ for all large primes $p$.

3. A refined Kaneko-Zagier conjecture: $\hat{A}$-MZV and $\hat{S}$-MZV

Further studies of the Kaneko–Zagier conjecture have been made by many authors [AHY, Jar1, Jar2, OSY21, Ros15, Ros, Yas19]. In this section, from their works we review a theory of $\hat{A}$-MZV and $\hat{S}$-MZV together with a conjectural relationship between them (which is called a refined version of the Kaneko–Zagier conjecture).

3.1. Supercongruences for multiple harmonic sums: an overview. Multiple harmonic sums satisfy mod $p^n$ congruences relations. A systematic study of these relations is due to Rosen [Ros15]. As a brief overview of his works, let us begin with a version of Rosen’s lifting conjecture [Ros15, Conjecture A].

Conjecture 3.1. Let $k$ be a positive integer and $p_1$ be a prime greater than $k + 1$. For a finite set $\{c_k \mid \text{wt}(k) = k\}$ of rational numbers, suppose that the congruence

$$\sum_{\text{wt}(k)=k} c_k H_{p-1}(k) \equiv 0 \mod p$$

holds for all primes $p \geq p_1$. Then, for each $n \geq 2$, there exists a prime $p_n$ and a finite set $\{c_k^{(l)} \mid 1 \leq l \leq n-1, \text{wt}(k) = k+l\}$ of rational numbers such that $p_n \geq p_{n-1}$ and the supercongruence

$$(3.1) \quad \sum_{\text{wt}(k)=k} c_k H_{p-1}(k) + \sum_{l=1}^{n-1} p^l \sum_{\text{wt}(k)=k+l} c_k^{(l)} H_{p-1}(k) \equiv 0 \mod p^n$$

holds for all primes $p \geq p_n$.

Roughly, Conjecture 3.1 says that mod $p$ congruences of $H_{p-1}(k)$’s, which hold for all but finitely many primes $p$, can be lifted into mod $p^n$ congruences of $p^l H_{p-1}(k)$’s for each $n$, which also hold for all but finitely many primes $p$ (note that the number of exceptions of primes in the latter congruence may be strictly bigger than the former ones for some $n$).
Let us illustrate two examples of lifts of mod $p$ congruences. For each positive integer $n$, Wolfstenholme’s theorem [Wol62], $H_{p-1}(1) \equiv 0 \mod p^2$, can be lifted into

\begin{equation}
H_{p-1}(1) + \sum_{l=0}^{n-2} p^l H_{p-1}(1 + l) \equiv 0 \mod p^n \quad (\forall p \gg 0 : \text{prime}),
\end{equation}

which is a special case of Corollary 4.3.3 in [Ros13]. Hoffman’s duality (2.2) extends to

\begin{equation}
\sum_{l=0}^{n-1} p^l \left( H_{p-1}^+(1, \ldots, 1, k) + H_{p-1}^+(1, \ldots, 1, k^\vee) \right) \equiv 0 \mod p^n \quad (\forall p : \text{prime})
\end{equation}

(see [Sek19]). Note that without fixing a basis, the way of extension is of course not unique. For example, one has

\[ H_{p-1}(1) + \frac{1}{3} p^2 H_{p-1}(2, 1) - \frac{1}{6} p^4 H_{p-1}(4, 1) - \frac{1}{9} p^5 H_{p-1}(4, 1, 1) \equiv 0 \mod p^6, \]

which again recovers Wolfstenholme’s theorem.

**Remark 3.2.** One can show that the injectivity of the $\mathcal{A}$-valued period map $\text{per}_A : \text{Fil}^0 \mathcal{P}^{nr} / \text{Fil}^1 \mathcal{P}^{nr} \rightarrow \mathcal{A}$, introduced by Rosen [Ros], implies Conjecture 3.1, where $\text{Fil}^*$ is a decreasing filtration coming from the Hodge filtration on algebraic de Rham cohomology. In our case, we consider $\mathcal{P}^{nr}$ as the ring of de Rham periods of mixed Tate motives over $\mathbb{Z}$. The map $\text{per}_A$ is an analogue of the period map, and is expected to be injective [Ros, Theorem 6.4].

### 3.2. $\hat{\mathcal{A}}$-MZV

To deal with congruences of type (3.1), Rosen [Ros15] introduces the $\mathbb{Q}$-algebra

\[ \mathcal{A}_n = \left( \prod_{p: \text{prime}} \mathbb{Z}/p^n \mathbb{Z} \right) / \left( \bigoplus_{p: \text{prime}} \mathbb{Z}/p^n \mathbb{Z} \right). \]

For each index $k$, let

\[ \zeta_{\mathcal{A}_n}(k) = \left( H_{p-1}(k) \mod p^n \right)_p \in \mathcal{A}_n \]

and set $p = \left( p \mod p^n \right)_p$. In $\mathcal{A}_n$, (3.1) can be written as an identity

\[ \sum_{\text{wt}(k)=k} c_k \zeta_{\mathcal{A}_n}(k) + \sum_{l=1}^{n-1} p^l \sum_{\text{wt}(k)=k+l} c_k^{(l)} \zeta_{\mathcal{A}_n}(k) = 0. \]

Relations among $\zeta_{\mathcal{A}_n}(k)$ are of particular interest and discussed in [MOS20, OSS].

As a completion of $\mathcal{A}_n$, Rosen [Ros15, Definition 3.2] defines the $\mathbb{Q}$-algebra $\hat{\mathcal{A}}$ to be the projective limit

\begin{equation}
\hat{\mathcal{A}} = \lim_{\leftarrow n} \mathcal{A}_n,
\end{equation}

\[ \hat{\mathcal{A}} = \left( \prod_{p: \text{prime}} \mathbb{Z}/p^n \mathbb{Z} \right) / \left( \bigoplus_{p: \text{prime}} \mathbb{Z}/p^n \mathbb{Z} \right). \]
where for each \( n \geq 1 \) the transition map \( \varphi_n : \mathcal{A}_{n+1} \to \mathcal{A}_n \) is induced from the natural projection \( \mathbb{Z}/p^{n+1}\mathbb{Z} \to \mathbb{Z}/p^n\mathbb{Z} \). Note that \( \hat{\mathcal{A}} \) is complete under the \( p \)-adic topology, where \( p = (p \mod p^n)_p \in \hat{\mathcal{A}} \). Any element of \( \hat{\mathcal{A}} \) is written as \( (a_{p,n + 1})_p \in \hat{\mathcal{A}} \) with \( (a_{p,n + 1})_p \in \mathcal{A}_n \) satisfying \( \varphi_n((a_{p,n + 1})_p) = (a_{p,n})_p \) for all \( n \geq 1 \). Then two elements \( (a_{p,n + 1})_p \) and \( (b_{p,n + 1})_p \) of \( \hat{\mathcal{A}} \) are identified if and only if there exists an increasing sequence \( \{p_n\}_{n \geq 1} \) of primes such that \( a_{p,n + 1} \equiv b_{p,n + 1} \mod p^n \) for all primes \( p \geq p_n \) and \( n \geq 1 \). We remark that there exists a natural surjective homomorphism (see [Ros15, §3.2])

\[
\prod_p \mathbb{Z}_p \to \hat{\mathcal{A}}.
\]

The following definition was first made by Rosen [Ros15] (we use Seki’s modification [Sek19]).

**Definition 3.3.** For an index \( k \), we define the \( \hat{\mathcal{A}} \)-MZV \( \zeta_{\hat{\mathcal{A}}}(k) \in \hat{\mathcal{A}} \) by

\[
\zeta_{\hat{\mathcal{A}}}(k) = \left( (H_{p-1}(k) \mod p^n)_p \right)_n
\]

and the \( \hat{\mathcal{A}} \)-MZSV \( \zeta^*_{\hat{\mathcal{A}}}(k) \in \hat{\mathcal{A}} \) by

\[
\zeta^*_{\hat{\mathcal{A}}}(k) = \left( (H^*_{p-1}(k) \mod p^n)_p \right)_n.
\]

For each weight \( k \), \( \hat{\mathcal{A}} \)-MZVs satisfy numerous relations of the form

\[
\sum_{l \geq 0} p^l \sum_{\text{wt}(k) = k + l} c_k^{(l)} \zeta_{\hat{\mathcal{A}}}(k) = 0
\]

with rational numbers \( c_k^{(l)} \). For example, the relations (3.2) and (3.3) are in \( \hat{\mathcal{A}} \) expressed as

\[
(3.5) \quad \zeta_{\hat{\mathcal{A}}}(1) + \sum_{l \geq 0} p^l \zeta_{\hat{\mathcal{A}}}(1 + l) = 0
\]

and

\[
(3.6) \quad \sum_{l \geq 0} p^l \left( \zeta^*_{\hat{\mathcal{A}}}(1, \ldots, 1, k) + \zeta^*_{\hat{\mathcal{A}}}(1, \ldots, 1, k^\circ) \right) = 0,
\]

respectively.

### 3.3. \( \tilde{S} \)-MZV.

As a counterpart of \( \hat{\mathcal{A}} \)-MZVs, for each index \( k \) we define

\[
\zeta^*_\tilde{S}(k) = \sum_{a = 0}^{\text{dep}(k)} (-1)^{\text{wt}(k_a)} \sum_{l \in \mathbb{Z}_{\geq 0}} t^{\text{wt}(l)} b\left( \begin{array}{c} k_a \\ l \end{array} \right) \zeta^*(k_a + l; T) \zeta^*(k^a; T) \in \mathcal{Z}[t]
\]

with the regularization \( \bullet \in \{*, \sqcup\} \). The above right side does not depend on \( T \) (see, for example, [OSY21, Proposition 2.3]). Hence, for each index \( k \) and \( \bullet \in \{*, \sqcup\} \),
the \( \zeta_\hat{S}(k) \) lies in the formal power series ring \( \mathbb{Z}[t] \) over \( \mathbb{Z} \). It was shown in [Jar2, Proposition 3.2.4] (see also [OSY21, Proposition 2.1]) that the equality
\[
\zeta_\hat{S}(k) \equiv \zeta_\hat{\mu}(k) \mod \pi i \mathbb{Z}[\pi i][t]
\]
holds for each index \( k \). Hence, the following definition is independent of the choice of the regularization \( \bullet \in \{\ast, /A_1\} \).

**Definition 3.4.** For an index \( k \), we define the \( \hat{S} \)-MZV \( \zeta_\hat{S}(k) \in \mathbb{Z}[\pi i][t] \) by
\[
\zeta_\hat{S}(k) = \zeta_\ast(k) \mod \pi i \mathbb{Z}[\pi i][t],
\]
where we set \( \mathbb{Z}[\pi i][t] = (\mathbb{Z}[\pi i]/\pi i \mathbb{Z}[\pi i])[t] \).

The \( \hat{S} \)-MZSV is defined by
\[
\zeta_\hat{S}(k_1, \ldots, k_d) = \sum_{\Box \text{ is either a comma } ', ' \text{ or a plus } '+'} \zeta_\hat{S}(k_1\Box \cdots \Box k_d).
\]

Note that the constant term of \( \zeta_\hat{S}(k) \) in \( t \) coincides with \( \zeta_S(k) \). Studies of the \( \hat{S} \)-MZV are initiated by Hirose, Rosen and Jarossay (he called \( \hat{S} \)-MZV, without taking modulo \( \pi i \), the \( \Lambda \)-adic adjoint MZV), independently. Relations among \( \hat{S} \)-MZVs of the form
\[
\sum_{l \geq 0} t^l \sum_{\text{wt}(k) = k + l} c_{k}^{(l)} \zeta_\hat{S}(k) = 0
\]
are particular interest in this study. For example, as a counterpart of (3.6), Hirose obtained
\[
(3.7) \sum_{l=0}^{\infty} t^l \left( \zeta_\hat{S}(1, \ldots, 1, k) + \zeta_\hat{S}(1, \ldots, 1, k^\prime) \right) = 0
\]
in his unpublished work.

### 3.4. \( \hat{A} \)-MZV vs. \( \hat{S} \)-MZV.

Similarly to the Kaneko–Zagier conjecture (Conjecture 2.3), there is a conjectural correspondence between \( \hat{A} \)-MZVs and \( \hat{S} \)-MZVs.

**Conjecture 3.5** (A refined version of the Kaneko–Zagier conjecture). *Let \( k \) be a positive integer. For rational numbers \( \{c_{k}^{(l)} \in \mathbb{Q} \mid \text{wt}(k) = k + l, \ l \geq 0\} \), we have*
\[
\sum_{l \geq 0} p^l \left( \sum_{\text{wt}(k) = k + l} c_{k}^{(l)} \zeta_\hat{A}(k) \right) = 0 \text{ in } \hat{A}
\]
\[
\iff \sum_{l \geq 0} t^l \left( \sum_{\text{wt}(k) = k + l} c_{k}^{(l)} \zeta_\hat{S}(k) \right) = 0 \text{ in } \mathbb{Z}[t].
\]
Similar statements with Conjecture 3.5 can be found in [Jar2, Conjecture 5.3.2], [Ros19, Conjecture 2.3] and [OSY21, Conjecture 4.3]. Several evidence of Conjecture 3.5 are known. The duality formulas (3.6) and (3.7) are one of examples. Also, a kind of double shuffle relations for both $\hat{A}$-MZVs and $\hat{S}$-MZVs in the same shape is obtained in [Jar2, OSY21].

We mention a relationship with the Kaneko–Zagier conjecture (Conjecture 2.3).

**Proposition 3.6.** Under the assumption that Conjecture 3.1 holds, Conjecture 3.5 implies Conjecture 2.3.

**Proof.** Assume that we have

$$\sum_{\text{wt}(k)=k} c_k^{(0)} \zeta_{\hat{A}}(k) = 0. \tag{3.8}$$

Conjecture 3.1 says that there exist rational numbers $c_k^{(l)}$ ($l \geq 1$) such that

$$\sum_{l \geq 0} p^l \sum_{\text{wt}(k)=k+l} c_k^{(l)} \zeta_{\hat{A}}(k) = 0. \tag{3.9}$$

Using Conjectures 3.5, we obtain

$$\sum_{l \geq 0} t^l \sum_{\text{wt}(k)=k+l} c_k^{(l)} \zeta_{\hat{S}}(k) = 0. \tag{3.10}$$

Comparing the constant terms of both sides, one has

$$\sum_{\text{wt}(k)=k} c_k^{(0)} \zeta_{\hat{S}}(k) = 0, \tag{3.11}$$

so, (3.8) $\Rightarrow$ (3.11). For the opposite implication (3.11) $\Rightarrow$ (3.8), Yasuda’s result [Yas16], stating that all MZVs of weight $k$ are $\mathbb{Q}$-linear combinations of $\mathcal{S}$-MZVs of weight $k$, determines a lift of (3.11) to (3.10), inductively (the same argument is used in the proof of [OSY21, Proposition 4.4]). Using Conjecture 3.5 and then applying to (3.9) the natural isomorphism $\hat{A}/p\hat{A} \cong \mathcal{A}$ given by $\zeta_{\hat{A}}(k) \mod p \mapsto \zeta_{\mathcal{A}}(k)$, we get (3.8). We complete the proof. \qed

4. $\hat{\mathbb{Q}}$-MZV

In this section, we introduce a $\hat{\mathbb{Q}}$-MZV and give a generalization of Theorem 2.8.

4.1. The $\mathbb{Q}$-algebra $\hat{\mathbb{Q}}$. Let us first extend the framework of $\mathbb{Q}$-MZVs.

For each $n \geq 1$ and a prime $p$, let $([p]^n)$ be the ideal of $\mathbb{Z}_{(p)}[q]$ generated by the polynomial $[p]^n$, where $\mathbb{Z}_{(p)}[q]$ denotes the polynomial ring in $q$ over the ring $\mathbb{Z}_{(p)}$ of
rational numbers whose denominators are not divisible by $p$. Consider the rings

$$Z_{p,n} = Z(p)[q]/([p]_q^n) \quad \text{and} \quad Q_n = \left( \prod_p Z_{p,n} \right) \bigg/ \left( \bigoplus_p Z_{p,n} \right),$$

where $p$ runs over all primes. Note that $Q = Q_1$. An element of $Q_n$ is of the form $(f_{p,n})_p$, where $p$ runs over all primes and $f_{p,n} \in Z_{p,n}$. Two elements $(f_{p,n})_p$ and $(g_{p,n})_p$ are identified if and only if $f_{p,n} = g_{p,n}$ for all but finitely many primes $p$. One can embed $Q[q]$ into $Q_n$ diagonally. Component-wise addition, multiplication and scalar multiplication by $Q[q]$ equip $Q_n$ with the structure of a $Q[q]$-algebra.

Similarly to the $Q$-algebra $\hat{A}$, we define the $Q[q]$-algebra $\hat{Q}$ to be the projective limit of the system of rings $\{Q_n\}$:

$$\hat{Q} = \lim_n Q_n,$$

where for each $n \geq 1$ the transition map $\varphi_n : Q_{n+1} \to Q_n$ is induced from the natural projection $Z_{p,n+1} \to Z_{p,n}$. It is endowed with the projective limit topology induced from the discrete topology on $Q_n$. We also have a natural surjective homomorphism

$$\prod_p Z_p \to \hat{Q},$$

where $Z_p = \lim_n Z_{p,n}$ denotes the ring of $[p]$-adic integers (cf. [Sek19, Lemma 2.3]).

Any element of $\hat{Q}$ is written as $((f_{p,n})_p)_n$ with $(f_{p,n})_p \in Q_n$ satisfying $\varphi_n((f_{p,n+1})_p) = (f_{p,n})_p$ for all $n \geq 1$. Then two elements $((f_{p,n})_p)_n$ and $((g_{p,n})_p)_n$ of $\hat{Q}$ are identified if and only if there exists an increasing sequence $\{p_n\}_{n \geq 1}$ of primes such that $f_{p,n} = g_{p,n}$ in $Z_{p,n}$ for all primes $p \geq p_n$ and $n \geq 1$.

Define the element $[p]$ of $\hat{Q}$ by

$$[p] = (([p] \mod [p]_q^n)_p)_n.$$

The continuous homomorphism $\hat{Q} \to Q_n$ induces $Q_n \cong \hat{Q}/[p]^n\hat{Q}$. The projective limit topology on $\hat{Q}$ coincides with the $[p]$-adic topology and $\hat{Q}$ is complete under the $[p]$-adic topology (cf. [Sek19, Lemma 2.5]).

4.2. Definition of $\hat{Q}$-MZV. We begin with the following lemma.

**Lemma 4.1.** Let $p$ be a prime and $p > m \geq 1$. For any $n \geq 1$, the $q$-integer $[m]$ is invertible in $Z_{p,n}$. More explicitly its inverse is given by

$$\frac{1}{[m]} \equiv [l]_q \sum_{j=0}^{n-1} (-q[\alpha]_{q[p]})^j \mod [p]^n,$$

where $l$ and $\alpha$ are the integers satisfying $p > l \geq 1, \alpha \geq 0$ and $ml - p\alpha = 1$. 
Proof. Using the relation $ml = 1 + p\alpha$, we see that $[m][l]_{q^n} = 1 + q[\alpha]_{q^n}[p]$. Hence we have

$$[m][l]_{q^n} \sum_{j=0}^{n-1} (-q[\alpha]_{q^n}[p])^j = 1 - (-q[\alpha]_{q^n}[p])^n \equiv 1 \mod [p]^n,$$

which completes the proof. \hfill \Box

From Lemma 4.1, the following definition makes sense.

**Definition 4.2.** For an index $k$ and $\bullet \in \{\emptyset, \star\}$, we define

$$\zeta^\bullet_{\hat{Q}}(k) = \left((H^\bullet_{p-1}(k; q) \mod [p]^n)_p\right)_n$$

and

$$\zeta^\bullet_{\hat{O}}(k) = \left((\overline{H}^\bullet_{p-1}(k; q) \mod [p]^n)_p\right)_n$$

as elements in $\hat{Q}$, where for an index $k = (k_1, \ldots, k_d)$, we set

$$H^\bullet_m(k; q) = \sum_{m \geq m_1 > \cdots > m_d > 0} \prod_{a=1}^d q_{m_1 \cdots m_d}^{m_a} \overline{H}^\bullet_{m}(k; q) = \sum_{m \geq m_1 > \cdots > m_d > 0} \prod_{a=1}^d q_{m_1 \cdots m_d}^{m_a}.$$

In the same vein with Remark 2.7, we call the above objects $\hat{Q}$-multiple zeta values (abbreviated by $\hat{Q}$-MZVs). The use of “bar” on $\zeta_{\hat{O}}$ seems confusing with the complex conjugate, but it comes into play in the study of relations later.

In what follows, similarly to §2.8, we prepare algebra maps $\phi_{\hat{A}} : \hat{Q} \to \hat{A}$ and $\phi_{\hat{S}} : \hat{O} \to \mathbb{C}[[t]]$, and then, give our main result stating that $\hat{A}$-MZVs and $\hat{S}$-MZVs are obtained as images of $\hat{Q}$-MZVs under these maps. Since the setting of $\phi_{\hat{S}}$ needs more spaces, we do this in the following two subsections and the proof of our main result is postponed to Appendix A.

4.3. **From $\hat{Q}$-MZV to $\hat{A}$-MZV.** The map $\phi_{\hat{A}}$ is defined in a similar manner to $\phi_{\hat{A}}$ in §2.8. If two polynomials $f(q)$ and $g(q)$ over $\mathbb{Z}_{(p)}$ satisfies $f(q) \equiv g(q) \mod [p]^n$, then $f(1) \equiv g(1) \mod p^n$. Therefore, there is the natural projection

$$Z_{p,n} \twoheadrightarrow \mathbb{Z}_{(p)}/p^n\mathbb{Z}_{(p)} \simeq \mathbb{Z}/p^n\mathbb{Z}$$

that sends $q$ to 1. This induces the continuous surjective algebra map

$$\phi_{\hat{A}} : \hat{Q} \twoheadrightarrow \hat{A}, \quad ((f_{p,n}(q) \mod [p]^n)_p)_n \longmapsto ((f_{p,n}(1) \mod p^n)_p)_n.$$

**Theorem 4.3.** For all index $k$ and $\bullet \in \{\emptyset, \star\}$, we have

$$\phi_{\hat{A}}(\zeta^\bullet_{\hat{Q}}(k)) = \phi_{\hat{A}}(\overline{\zeta}^\bullet_{\hat{O}}(k)) = \zeta^\bullet_{\hat{A}}(k).$$

**Proof.** This is immediate from the identity

$$\phi_{\hat{A}}\left(((m)^{-1} \mod [p]^n)_p\right)_n = ((m^{-1} \mod p^n)_p)_n$$
for any \( m \in \{1, 2, \ldots, p - 1\} \).

\[ \square \]

4.4. From \( \hat{Q} \)-MZV to \( \hat{S} \)-MZV. The map \( \phi_\mathcal{S} \) is defined to be the composition of two algebra maps \( \hat{\lim} \) and \( \hat{\ev} \), as in the same vein as \( \phi_\mathcal{S} \) in §2.8.

First, let us define \( \hat{\ev} \). For a prime \( p \) and \( n \geq 1 \), set

\[
Z_{p,n}^{\text{an}} = Q(\zeta_p)[[t]]/(t^n) \quad \text{and} \quad \mathcal{Q}_n^{\text{an}} = \left( \prod_{p \text{ prime}} Z_{p,n}^{\text{an}} \right) / \left( \bigoplus_{p \text{ prime}} Z_{p,n}^{\text{an}} \right).
\]

We also write \( (f_{p,n})_p \) for an element of \( \mathcal{Q}_n^{\text{an}} \), where \( p \) runs over all primes and \( f_{p,n} \in Z_{p,n}^{\text{an}} \). We apply the same construction with \( \hat{Q} \) to

\[
\hat{\mathcal{Q}}_n^{\text{an}} = \hat{\lim}_n \mathcal{Q}_n^{\text{an}},
\]

where the transition map \( \mathcal{Q}_n^{\text{an}} \to \mathcal{Q}_{n+1}^{\text{an}} \) is induced by the natural projection \( Z_{p,n+1}^{\text{an}} \to Z_{p,n}^{\text{an}} \). The \( \mathbb{Q} \)-algebra \( \hat{\mathcal{Q}}_n^{\text{an}} \) is complete under the \( t \)-adic topology, where

\[
t = \left( (t \mod t^n)_p \right)_n \in \hat{\mathcal{Q}}_n^{\text{an}}.
\]

There exists a unique formal power series \( q_m(t) \in \mathcal{Q}(\zeta_m)[[t]] \) such that

\[
q_m(0) = e^{\frac{2\pi i}{m}} \quad \text{and} \quad [m]_{q_m(t)} = t.
\]

For example, solving the above equations, one gets

\[
q_m(t) = e^{\frac{2\pi i}{m}} + (1 - e^{-\frac{2\pi i}{m}}) \frac{t}{m} + O(t^2).
\]

Alternatively, the power series \( q_m(t) \) can be viewed as an inverse function of \( t = [m]_q \), which is holomorphic in a neighborhood of \( t = 0 \) because \( dt/dq \neq 0 \) at \( q = e^{2\pi i/m} \).

See Remark A.4 for the explicit Taylor expansion. For each prime \( p \), we use the power series \( q_p(t) \) to get the \( \mathbb{Z}(p) \)-homomorphism

\[
Z_{p,n} \rightarrow Z_{p,n}^{\text{an}}, \quad f(q) \mod [p]^n \mapsto f(q_p(t)) \mod t^n.
\]

It induces the continuous \( \mathbb{Q} \)-algebra map

\[
\hat{\ev} : \hat{\mathcal{Q}} \rightarrow \hat{\mathcal{Q}}^{\text{an}}, \quad ((f_{p,n}(q) \mod [p]^n)_p)_n \mapsto ((f_{p,n}(q_p(t)) \mod t^n)_p)_n.
\]

Secondly, we introduce \( \hat{\lim} \). Let \( \mathcal{O}_n^{\text{an}} \) be the \( \mathbb{Q} \)-subalgebra of \( \prod_p Z_{p,n}^{\text{an}} \) given by

\[
\mathcal{O}_n^{\text{an}} = \left\{ \left( \sum_{l=0}^{n-1} z_{p,l} t^l \mod t^n \right)_p \in \prod_p Z_{p,n}^{\text{an}} \mid \lim_{p \to \infty} z_{p,l} \text{ converges for all } 0 \leq l \leq n - 1 \right\}.
\]

Note that \( \bigoplus_p Z_{p,n}^{\text{an}} \subset \mathcal{O}_n^{\text{an}} \subset \prod_p Z_{p,n}^{\text{an}} \). We define the \( \mathbb{Q} \)-subalgebra \( \hat{\mathcal{O}}_n^{\text{an}} \) of \( \hat{\mathcal{Q}}_n^{\text{an}} \) by

\[
\hat{\mathcal{O}}_n^{\text{an}} = \hat{\lim}_n \left( \mathcal{O}_n^{\text{an}} / \bigoplus_p Z_{p,n}^{\text{an}} \right).
\]
The transition map \( \mathcal{O}^\text{an}_{n+1}/\bigoplus_p Z_{p,n+1}^\text{an} \to \mathcal{O}/\bigoplus_p Z_{p,n}^\text{an} \) is also induced by the natural projection \( Z_{p,n+1}^\text{an} \to Z_{p,n}^\text{an} \). It can be shown that \( \hat{\mathcal{O}}^\text{an} \) is a closed subset of \( \hat{\mathcal{O}}^\text{an} \). We note that any element \( z \) of \( \hat{\mathcal{O}}^\text{an} \) is written in the form

\[
z = (\sum_{l=0}^{n-1} z_{p,l}^{(n)} t^l \mod t^n)_p \mod \bigoplus_p Z_{p,n}^\text{an}
\]

with convergent sequences \( \{z_{p,l}^{(n)}\}_p \) satisfying the condition that there exists an increasing sequence \( \{p_n\}_{n \geq 1} \) of primes such that, for all \( n \geq 1 \) and primes \( p \geq p_n \), the equality \( z_{p,l}^{(n+1)} = z_{p,l}^{(n)} \) holds for each \( l \in \{0, 1, \ldots, n-1\} \). Taking \( p \to \infty \) we see that \( \lim_{p \to \infty} z_{p,l}^{(n)} = \lim_{p \to \infty} z_{p,l}^{(n)} \) for all \( 0 \leq l < n \). Set \( z_l = \lim_{p \to \infty} z_{p,l}^{(n)} \) for \( l \geq 0 \), which is independent on the choice of \( n \) greater than \( l \). Thus we obtain the \( \mathbb{Q} \)-algebra map

\[
\hat{\lim} : \hat{\mathcal{O}}^\text{an} \longrightarrow \mathbb{C}[[t]], \quad z \mapsto \sum_{t \geq 0} z_t t^l.
\]

It is continuous with respect to the \( t \)-adic topology on \( \mathbb{C}[[t]] \).

Finally, we define \( \phi_{\hat{\mathcal{O}}} \). Let us denote by \( \hat{\mathcal{O}} \) the closed \( \mathbb{Q} \)-subalgebra of \( \hat{\mathcal{O}} \) given by

\[
\hat{\mathcal{O}} = \{ z \in \hat{\mathcal{O}} \mid ev(z) \in \hat{\mathcal{O}}^\text{an} \} = ev^{-1}(\hat{\mathcal{O}}^\text{an})
\]

The map \( \phi_{\hat{\mathcal{O}}} \) is then defined by

\[
\phi_{\hat{\mathcal{O}}} = \hat{\lim} \circ \hat{ev} : \hat{\mathcal{O}} \longrightarrow \mathbb{C}[[t]],
\]

which is a continuous \( \mathbb{Q} \)-algebra map. It is explicitly described as follows. Let \( f = ((f_{p,n}(q) \mod [p]^n)_p)_n \) be an element of \( \hat{\mathcal{O}} \). Set \( f_{p,n}(q_p(t)) = \sum_{l=0}^{n-1} z_{p,l}^{(n)} t^l + O(t^n) \). Then one has \( \phi_{\hat{\mathcal{O}}}(f) = \sum_{l \geq 0} z_l t^l \) with \( z_l = \lim_{p \to \infty} z_{p,l}^{(n)} \) (\( n > l \)).

**Theorem 4.4.** For any index \( k \) and \( \bullet \in \{\emptyset, \ast\} \), we have \( \zeta_{\hat{\mathcal{O}}}^\ast(k) \in \hat{\mathcal{O}} \) and

\[
(4.2) \quad \phi_{\hat{\mathcal{O}}}(\zeta_{\hat{\mathcal{O}}}^\ast(k)) = \hat{\xi}(k)
\]

where \( \hat{\xi}(k), \hat{\xi}^\ast(k) \in \mathcal{Z}[[\pi]] \) are given by

\[
\hat{\xi}(k) = \sum_{\text{dep}(k)} (-1)^{wt(k_a)} \sum_{t \in \mathbb{Z}_{\geq 0}^a} \xi^{ wt(t)} \frac{b(k_a)}{l} \xi^\ast \left( \frac{k_a + l}{2} \right) \zeta^\ast \left( k_a; -\frac{\pi i}{2} \right)
\]

and

\[
\hat{\xi}^\ast(k_1, \ldots, k_d) = \sum_{\square \text{ is either a comma }, \ast\text{, or a plus } +} \hat{\xi}(k_1 \square \cdots \square k_d).
\]

Also, \( \overline{\zeta_{\hat{\mathcal{O}}}}(k) \) and \( \overline{\zeta_{\hat{\mathcal{O}}}}(k) \) belong to \( \hat{\mathcal{O}} \) and it holds that

\[
(4.3) \quad \phi_{\hat{\mathcal{O}}}(\overline{\zeta_{\hat{\mathcal{O}}}}(k)) = \overline{\xi}(k) \quad \text{and} \quad \phi_{\hat{\mathcal{O}}}(\overline{\zeta_{\hat{\mathcal{O}}}}(k)) = \overline{\xi}(k),
\]
where the bar on the right sides means taking the complex conjugate of each coefficient in a formal power series over \( \mathbb{C} \). In particular, for any index \( k \) and \( \bullet \in \{ \emptyset, \star \} \), we have

\[
\phi_\mathcal{S}(\zeta_\mathcal{Q}(k)) \equiv \phi_\mathcal{S}(\zeta_\mathcal{Q}(\kappa)) \equiv \zeta_\mathcal{S}(k) \mod \pi i \mathbb{Z}[\pi i][[t]].
\]

Our proof of Theorem 4.4 can be found in Appendix A.

Remark 4.5. Similarly to the map \( \text{ev} \), one can prove the injectivity of \( \hat{\text{ev}} \) as follows.

For a rational function \( f(q) \) in \( q \) over \( \mathbb{Z}(p) \) whose denominator is coprime to \( [p] \), it suffices to show that if \( f(q^p(t)) \equiv 0 \mod t^n \), then \( f(q) \equiv 0 \mod [p]^n \). Since \( q^p(t) - e^{2\pi i/p}p \equiv 0 \mod t \), we have \( f(q^p(t))/f(q(t) - e^{2\pi i/p})n \in \mathbb{Q}(\zeta^p)[[t]] \). Hence \( \frac{d}{dt}f(q^p(t)) \equiv 0 \mod t \), which shows that \( e^{2\pi i/p} \) is zero of \( f(q) \) of multiplicity \( n \).

Notice that the congruence in question is stable under the action of \( \text{Gal}(\mathbb{Q}(\zeta^p)/\mathbb{Q}) \).

Thus, all primitive \( p \)-th roots of unity are zero of \( f(q) \) of multiplicity \( n \). Since

\[
[p] = \prod_{a=1}^{p-1} (q - e^{2\pi ia/p}),
\]

we conclude \( f(q) \equiv 0 \mod [p]^n \).

4.5. Application. Let us illustrate an application to the study of relations of \( \hat{A} \)-MZVs and \( \hat{S} \)-MZVs. We extend Andrews’ relation (2.12) to \( \hat{Q} \)-MZVs and deduce corresponding relations for \( \hat{A} \)-MZVs and \( \hat{S} \)-MZVs.

An extension of Andrews’ relation (2.12) is as follows.

**Proposition 4.6.** We have

\[
\zeta_\hat{Q}(1) - \frac{p - 1}{2}(1 - q) + \frac{1}{2} \sum_{l \geq 1} [p]^l \zeta_\hat{Q}(1 + l) = 0.
\]

**Proof.** As a rational function in \( q \), it is shown in the proof of Theorem 1 in [SP07] that we have the identities

\[
H_{p-1}(1; q) - \frac{p - 1}{2}(1 - q) = \frac{1 - q(1 - q^p)}{2} \sum_{m=1}^{p-1} \frac{q^m}{(1 - q^m)(q^m - q^p)}
\]

\[
= -\frac{1}{2} [p] \sum_{m=1}^{p-1} \frac{q^m}{[m] ([m] - [p])^{-1}}.
\]

Using

\[
\frac{1}{[m] - [p]} = \sum_{l=0}^{n-1} \frac{1}{[m] [m+1]} [p]^l \mod [p]^n,
\]

we obtain the desired formula. \( \square \)

To apply the map \( \phi_\mathcal{F} \), we note

\[
\phi_\mathcal{F}([p]) = \Lambda
\]
holds for $\mathcal{F} = \mathcal{A}$ and $\mathcal{S}$, where $\Lambda$ is given by
\begin{equation}
\Lambda = \begin{cases} 
p & (\mathcal{F} = \mathcal{A}), 
t & (\mathcal{F} = \mathcal{S}). \end{cases}
\end{equation}
Using Proposition A.2 below, for $\mathcal{F} \in \{\mathcal{A}, \mathcal{S}\}$, we have
\[ \hat{\phi}_F(q) = 1 \]
and
\[ \hat{\phi}_S(p(1-q)) = -2\pi i, \quad \hat{\phi}_A(p(1-q)) = 0. \]
Now, applying $\hat{\phi}_S$ to Proposition 4.6, we obtain
\[ \hat{\xi}(1) + \pi i + \frac{1}{2} \sum_{l \geq 1} t^l \hat{\xi}(1+l) = 0, \]
which gives
\[ \zeta_S(1) + \sum_{l \geq 0} t^l \zeta_S(1+l) = 0. \]
On the other hand, applying $\hat{\phi}_A$ to Proposition 4.6, we get (3.5), which is the same shape with the above.

Remark 4.7. One of key ingredients of the study of relationships between $\hat{\zeta}_A(k)$ and $\hat{\zeta}_S(k)$ is the formula
\[ H_{p-1}(k) = \sum_{a=0}^{\text{dep}(k)} (-1)^{\text{wt}(k_a)} \sum_{t \in \mathbb{Z}_{\geq 0}} p^{\text{wt}(t)} b\left(\binom{k_a}{l}\right) \zeta_{p,\text{De}}^\eta(k_a + l) \zeta_{p,\text{De}}^\eta(k_a), \]
expressing the multiple harmonic sum $H_{p-1}(k)$ in terms of Deligne’s $p$-adic multiple zeta values (see [Fur07, Definition 2.7] for the definition of $\zeta_{p,\text{De}}^\eta(k)$, where they use the opposite convention, namely, our $\zeta_{p,\text{De}}^\eta(k)$ corresponds to their $\zeta_{p,\text{De}}^\eta(k)$). Remark that the above formula was obtained by Akagi-Hirose-Yasuda [AHY] and first proved by Jarossay [Jar1]. It is of interest to find a $q$-analogue of the above formula.

5. Reversal, Duality and Cyclic sum formulas for $\hat{\mathcal{Q}}$-MZVs

In this section, we will see that reversal, duality and cyclic sum formulas for both $\hat{\mathcal{A}}$-MZVs and $\hat{\mathcal{S}}$-MZVs can be extended to $\hat{\mathcal{Q}}$-MZVs. Proofs use well-known techniques in $q$-analogues, so are postponed to Appendix B.

5.1. Reversal formula. Since $q^p = 1 - (1 - q)[p]$, for all primes $p$ and $n \geq 1$, we have $(q^p)^{-1} \equiv \sum_{j=0}^{n-1} ((1 - q)[p])^j \mod [p]^n$. Hence, letting
\[ q^\pm p = (((q^p)^{\pm 1} \mod [p]^n)_p)_n \in \hat{\mathcal{Q}}, \]
we obtain
\[ q^p = 1 - (1 - q)[p], \quad q^{-p} = \sum_{l \geq 0} ((1 - q)[p])^l. \]

**Theorem 5.1.** For any index \( k \) and \( \bullet \in \{\emptyset, \star\} \), it holds that
\[
\zeta_\hat{Q}(k) = (-q^{-p})^{\text{wt}(k)} (q^p)^{\text{dep}(k)} \sum_{l \in \mathbb{Z}_{\geq 0}} ((q^{-p}[p])^{\text{wt}(l)} b\left(\frac{k}{l}\right) \zeta_\hat{Q}(k + l)).
\]

**Corollary 5.2.** For all index \( k \), \( \bullet \in \{\emptyset, \star\} \) and \( F \in \{A, S\} \), we have
\[
\zeta_\hat{F}(k) = (-1)^{\text{wt}(k)} \sum_{l \in \mathbb{Z}_{\geq 0}} \Lambda^{\text{wt}(l)} b\left(\frac{k}{l}\right) \zeta_\hat{F}(k + l),
\]
where \( \Lambda \) is defined by (4.4). We also have
\[
\overline{\zeta_\hat{\star}(k)} = (-1)^{\text{wt}(k)} \sum_{l \in \mathbb{Z}_{\geq 0}} \Lambda^{\text{wt}(l)} b\left(\frac{k}{l}\right) \overline{\zeta_\hat{\star}(k + l)},
\]
where the bar on the left means the complex conjugate.

**Remark 5.3.** The mod \([p]\) version of Theorem 5.1 is proved in [HHT17, Theorem 3.1] with the same method. Corollary 5.2 for \( F = A \) is proved in [Ros15, Theorem 4.1]. Corollary 5.2 for \( \zeta_\hat{S} \) is a special case of the shuffle relation, which can be found in, e.g., [Jar2] and [OSY21].

### 5.2. Duality formula.
For all odd primes \( p \) and \( n \geq 1 \), we have
\[
q^{p(p+1)/2} = (1 - (1 - q)[p])^{(p+1)/2} \equiv \sum_{l=0}^{n-1} \left(\frac{p+1}{l}\right) ((1 - q)[p])^l \mod [p]_p.
\]

Let
\[
q^{p(p+1)/2} = ((q^{p(p+1)/2} \mod [p]_p)_n) \in \hat{Q}.
\]

**Theorem 5.4.** For any index \( k \), it holds that
\[
q^{p(p+1)/2} \sum_{l \geq 0} [p]^l \zeta_\hat{Q}(\{1\}^l, k) + \sum_{l \geq 0} (q^{-p}[p])^l \overline{\zeta_\hat{Q}(\{1\}^l, k^\vee)} = 0,
\]
where \( \{1\}^l = 1, \ldots, 1 \).

**Corollary 5.5.** Let \( k \) be an index. We have
\[
\sum_{l \geq 0} \Lambda^l \zeta_\hat{F}(\{1\}^l, k) + \sum_{l \geq 0} \Lambda^l \zeta_\hat{F}(\{1\}^l, k^\vee) = 0
\]
for $\mathcal{F} = \mathcal{A}$ and $\mathcal{S}$, where $\Lambda$ is given by (4.4), and

\begin{equation}
\sum_{l \geq 0} t^l \hat{\xi}^*([1]^l, k) + \sum_{l \geq 0} \hat{\xi}^*([1]^l, k^l) = 0.
\end{equation}

Remark 5.6. The duality formula (5.1) for $\hat{A}$-MZVs is proved by Seki [Sek19], and its proof is simplified by Shuji Yamamoto. Our proof of Theorem 5.4 is a $q$-analogue of the simplified proof. We thank Shin-ichiro Seki and Shuji Yamamoto for informing their results to us. The duality formula (5.2) is announced by Minoru Hirose.

5.3. Cyclic sum formula. Let $\mathfrak{S}_d$ be the symmetric group on a set of $d$ elements. The subgroup of $\mathfrak{S}_d$ generated by the cyclic permutation $\sigma = (1, 2, \ldots, d)$ acts on the set of indices of weight $k$ and depth $d$ by $\sigma(k_1, k_2, \ldots, k_d) = (k_2, \ldots, k_d, k_1)$. We denote the set of orbits of the action by $\Pi(k, d)$. For an orbit $\alpha \in \Pi(k, d)$ we denote its cardinality by $|\alpha|$.

Theorem 5.7. For any orbit $\alpha \in \Pi(k, d)$ it holds that

\begin{equation}
\sum_{k \in \alpha} \sum_{s=0}^{k_1-2} \zeta_{\hat{Q}}(k_1 - s, k^l, s + 1)
= \sum_{k \in \alpha} \zeta_{\hat{Q}}(k_1 + 1, k^l) + \sum_{k \in \alpha} \sum_{l \geq 0} (q^{-p}[p])^l \left\{ \zeta_{\hat{Q}}(k^l, k_1, l + 1) + \zeta_{\hat{Q}}(k^l, k_1 + l + 1) \right\}
+ (1 - q) \sum_{k \in \alpha} \sum_{l \geq 0} (q^{-p}[p])^l \zeta_{\hat{Q}}(k^l, k_1 + l)
\end{equation}

and

\begin{equation}
\sum_{k \in \alpha} \sum_{s=0}^{k_1-2} \zeta_{\hat{Q}}^*(k_1 - s, k^l, s + 1)
= \frac{k}{d} |\alpha| \zeta_{\hat{Q}}^*(k + 1) + |\alpha| \sum_{j=1}^{d} \left( \frac{k}{j} - 1 \right) \left( \frac{d}{j} \right) (1 - q)^j \zeta_{\hat{Q}}^*(k + 1 - j)
+ \sum_{k \in \alpha} \sum_{l \geq 0} (q^{-p}[p])^l \zeta_{\hat{Q}}^*(k^l, k_1, l + 1).
\end{equation}

Corollary 5.8. For any $\alpha \in \Pi(k, d)$ and $\mathcal{F} \in \{\mathcal{A}, \mathcal{S}\}$ we have

\begin{equation}
\sum_{k \in \alpha} \sum_{s=0}^{k_1-2} \zeta_{\hat{F}}(k_1 - s, k^l, s + 1)
= \sum_{k \in \alpha} \zeta_{\hat{F}}(k_1 + 1, k^l) + \sum_{k \in \alpha} \sum_{l \geq 0} \Lambda^l \left( \zeta_{\hat{F}}(k^l, k_1, l + 1) + \zeta_{\hat{F}}(k^l, k_1 + l + 1) \right)
\end{equation}
and
\[ \sum_{k \in \alpha} \sum_{s=0}^{k_1-2} \zeta^*_F(k_1-s, k_1, s+1) = \frac{k}{d} |\alpha| \zeta^*_F(k_1+1) + \sum_{k \in \alpha} \sum_{l \geq 0} \Lambda^l \zeta^*_F(k_1, k_1, l+1), \]
where \( \Lambda \) is defined by (4.4). The above equality with \( \zeta^*_F \) and \( \Lambda \) replaced by \( \hat{\zeta}^* \) and \( \tau \), respectively, also holds for \( \bullet \in \{\emptyset, \ast\} \).

Remark 5.9. Our proof of Theorem 5.7 is a \( q \)-analogue of the proof of Corollary 5.8 for \( F = A \) due to Kawasaki [Kaw19] (see also [KO20]). Corollary 5.8 for \( F = S \) is shown in [HMO] and Corollary 5.8 for \( \hat{\zeta}^* \) mod \( \tau \) is announced by Nobuo Sato and Minoru Hirose.

6. Discussions on dimensions

6.1. Enumeration of relations among \( Q \)-MZVs. This subsection discusses relations of \( \zeta_Q(k) \)'s of the form (2.11), based on some experimental works.

For \( k \geq 1 \), we denote by \( \mathbb{I}_k \) the set of all indices of weight \( k \). Consider the \( Q \)-vector space \( Z_k^O \) spanned by the set
\[ \{ p^h(1-q)^j \zeta_Q(k) \mid 0 \leq h \leq j \leq k, \ k \in \mathbb{I}_{k-j} \}, \]
which is a \( Q \)-vector subspace of the \( \mathbb{Q}[p] \)-module generated by elements \( (1-q)^j \zeta_Q(k) \) of weight \( k \). For example, the space \( Z_2^O \) is generated by
\[ \zeta_Q(2), \zeta_Q(1, 1), (1-q)\zeta_Q(1), p(1-q)\zeta_Q(1), (1-q)^2, p(1-q)^2, p^2(1-q)^2. \]

We let \( Z_0^O = \mathbb{Q} \) as usual. The reason why we consider the \( Q \)-vector space \( Z_k^O \), not the \( \mathbb{Q}[p] \)-module, is that the whole space
\[ Z^O = \sum_{k \geq 0} Z_k^O \]
with the product given by the \( q \)-stuffle product (see [Bra05-1]) is a subalgebra of \( O \) defined in §2.8. Moreover, by Theorem 2.8 (and [Hir20, Proposition 16]), we have
\[ \phi_A(Z_k^O) = Z_k^A \text{ and } \phi_S(Z_k^O) = Z_k \oplus \pi Z_{k-1}. \]

Our numerical implementation (by [PARI]) is as follows. Let us fix a finite set \( S \) of primes. For each index \( k \) and \( 0 \leq h \leq j \), we first compute a polynomial \( n(h, j, k; q) \in \mathbb{Q}[q]/( \prod_{p \in S} [p] ) \) such that \( n(h, j, k; q) \equiv p^h(1-q)^j H_{p-1}(k; q) \mod [p] \) for all \( p \in S \) (use the Chinese remainder theorem), and then, find numerical \( \mathbb{Q} \)-linear relations among numerical values \( n(h, j, k; q) \)'s at \( q \) being a fixed transcendental number. These numerical data provide possible \( \mathbb{Q} \)-linear relations of the generator of \( Z_k^O \), and in this way, we can count the number of all linearly independent (possible) relations over \( \mathbb{Q} \). For simplicity, letting \( V_k = (1-q)Z_{k-1}^O + p(1-q)Z_{k-1}^O \subset Z_k^O \), we
below give a numerical dimension of
\[ \tilde{Z}_k^Q = \mathcal{Z}_k^Q / V_k. \]

### Table 1. Table of numerical dimensions

| \( k \) | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|----|----|----|----|----|----|----|----|----|----|----|----|----|
| \( \dim_Q \tilde{Z}_k^Q \) | 0  | 0  | 1  | 0  | 2  | 1  | 3  | 4  | 5  | 10 | 11 | 19 |
| \( \dim_Q Z_k^A \)   | 0  | 0  | 1  | 0  | 1  | 1  | 1  | 2  | 2  | 3  | 4  | 5  |

From the above table, since \( \phi_A(V_k) = \{0\} \) and \( \phi_S(V_k) \subset \pi_i\mathcal{Z}_{k-1} \), we see that up to weight 4 all linear relations among \( A \)-MZVs and \( S \)-MZVs are obtained from linear relations of \( p^h(1-q)^k \zeta_Q(k) \)'s. In weight 5, there is a relation which does not come from relations of \( \zeta_Q(k) \)'s. Such relation is already detected in [BTT18, §3.4]; for \( F \in \{A, S\} \), it is

\[(6.1) \quad \zeta_F(4, 1) - 2\zeta_F(3, 1, 1) = 0.\]

In other words, we expect that \( \zeta_Q(4, 1) - 2\zeta_Q(3, 1, 1) \not\in (1-q)\mathcal{Z}_5^Q + p(1-q)\mathcal{Z}_4^Q \).

**Examples of relations.** Using results we obtained in §5, we illustrate some examples of explicit relations and compute upper bounds of the dimension of \( \tilde{Z}_k^Q \) for \( k = 1, 2, 3 \). We remark that for each \( k \geq 1 \) there exists a polynomial \( c_k(x) \in \mathbb{Q}[x] \) of degree at most \( k \) such that \( \zeta_Q(k) = c_k(p)(1-q)^k \) (see, e.g., [Zha16, Corollary 9.5.5] and [BTT18, Remark 2.3]).

In weight 1, the identity (2.12) shows

\[(6.2) \quad \zeta_Q(1) \in V_1 = (1-q)\mathcal{Z}_0^Q + p(1-q)\mathcal{Z}_0^Q, \]

so \( \dim \tilde{Z}_1^Q = 0 \).

In weight 2, a generator of \( \tilde{Z}_2^Q \) is given by \( \{\zeta_Q(2), \zeta_Q(1, 1)\} \) and these satisfy

\[(6.3) \quad 0 = \zeta_Q(2) + \frac{p^2 - 1}{12} (1-q)^2, \]

\[0 = 2\zeta_Q(2) + \zeta_Q(1, 1) + (1-q)\zeta_Q(1), \]

where the last relation is obtained from Theorem 5.7 for the case \( k = d = 1 \). These relations imply \( \dim \tilde{Z}_2^Q = 0 \).

In weight 3 we get

\[0 = \zeta_Q(3) - \frac{p^2 - 1}{24} (1-q)^3, \]

\[0 = \zeta_Q(2, 1) + \zeta_Q(1, 2) + \zeta_Q(1, 1, 1) + (1-q)\zeta_Q(1, 1), \]

\[0 = \zeta_Q(3) + \zeta_Q(2, 1) + \zeta_Q(1, 2) + (1-q)\zeta_Q(2) + \frac{p^2 - 1}{12} (1-q)^2\zeta_Q(1), \]

\[0 = \zeta_Q(3) + \zeta_Q(2, 1) + \zeta_Q(1, 2) + (1-q)\zeta_Q(2) + \frac{p^2 - 1}{12} (1-q)^2\zeta_Q(1), \]
where the second relation is the case $k = d = 2$ in Theorem 5.7 modulo $[p]$ and the last relation can be deduced from (6.3) by multiplying by $\zeta_Q(1)$ and using the $q$-stuffle product

$$\zeta_Q(k_1)\zeta_Q(k_2) = \zeta_Q(k_1, k_2) + \zeta_Q(k_2, k_1) + \zeta_Q(k_1 + k_2) + (1 - q)\zeta_Q(k_1 + k_2 - 1).$$

Hence, one gets $\dim \tilde{Z}_3^Q \leq 1$.

**Remark 6.1.** Let us count the number of linearly independent relations obtained from the duality formula (2.7) and the $q$-stuffle product. For this, define the *stuffle-star product* $\star : \mathfrak{H}^1 \otimes \mathfrak{H}^1 \to \mathfrak{H}^1$ inductively by

$$y_k w \star y_l w' = y_k (w \star y_l w') + y_l (y_k w \star w') - y_{k+l} (w \star w')$$

for $w, w' \in \mathfrak{H}^1$ and $k, l \geq 1$, with the initial condition $w \star 1 = w = 1 \star w$. By the $q$-stuffle-star product (see [BTT18, §3.2] for the definition), for indices $k$ and $l$ with $\text{wt}(k) + \text{wt}(l) = k$, it holds that

$$\zeta_\star^Q(y_k)\zeta_\star^Q(y_l) - \zeta_\star^Q(y_k \star y_l) \in (1 - q)\mathbb{Z}_k^O,$$

where $\zeta_\star^Q$ is regarded as a $\mathbb{Q}$-linear map that sends $y_k$ to $\zeta_\star^Q(k)$. Hence, by (2.7), for any indices $k$ and $l$ with $\text{wt}(k) + \text{wt}(l) = k$, one obtains

$$\zeta_\star^Q(y_k \star y_l - (-1)^k y_k \star y_l) \in (1 - q)\mathbb{Z}_k^O.$$

Furthermore, using (6.2), for any index $k$ of weight $k - 1$, we see that

$$\zeta_\star^Q(y_1 \star y_k) \in V_k.$$

Now consider the $\mathbb{Q}$-vector subspace of $\mathfrak{H}^1_k = \langle y_k \mid k \in \mathbb{I}_k \rangle_{\mathbb{Q}}$ given by

$$\mathfrak{R}_k = \left\langle y_k \star y_l - (-1)^k y_k \star y_l \mid (k, l) \in \bigcup_{t=1}^{k-1} \mathbb{I}_t \times \mathbb{I}_{k-t} \right\rangle_{\mathbb{Q}}$$

$$+ \langle y_1 \star y_k \mid k \in \mathbb{I}_{k-1} \rangle_{\mathbb{Q}} + \langle y_k + (-1)^{\text{wt}(k)} y_k \star y_k \mid k \in \mathbb{I}_k \rangle_{\mathbb{Q}}.$$

Since $\zeta_\star^Q(w) \in V_k$ for any $w \in \mathfrak{R}_k$, it follows that

$$\dim \tilde{Z}_k^O \leq \dim \mathfrak{H}^1_k / \mathfrak{R}_k.$$

The exact dimension of the right side can be computed up to certain weights and the list, which coincides with the above numerical dimension of $\tilde{Z}_k^O$, is as follows.

**Table 2.** Table of numerical dimensions

| $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|-----|---|---|---|---|---|---|---|---|---|----|----|----|
| $\dim _\mathbb{Q} \mathfrak{H}^1_k / \mathfrak{R}_k$ | 0 | 0 | 1 | 0 | 2 | 1 | 3 | 4 | 5 | 10 | 11 | 19 |
6.2. Variants of Q-MZVs. In this subsection, we introduce variants of \( \zeta_Q(k) \) and discuss how we obtain (6.1) from our theory of Q-MZVs.

For an index \( k = (k_1, \ldots, k_d) \) and \( s = (s_1, \ldots, s_d) \in \mathbb{Z}_{\geq 0}^d \), we set
\[
H_m(k; s; q) = \sum_{m \geq m_1 > \ldots > m_d > 0} \prod_{a=1}^d q^{a_m} a_m^{k_a},
\]
and define
\[
\zeta_Q(k; s) = (H_{p-1}(k; s; q) \mod [p])_p \in \mathbb{Q}.
\]
Note that \( \zeta_Q(k_1, \ldots, k_d; k_1-1, \ldots, k_d-1) = \zeta_Q(k_1, \ldots, k_d) \) and \( \zeta_Q(k_1, \ldots, k_d; 1, \ldots, 1) = \zeta_Q(k_1, \ldots, k_d) \). For \( k \geq 1 \), let \( \mathcal{Z}_k^Q \) be the \( \mathbb{Q} \)-vector space spanned by the set
\[
\{ p^h(1-q)_j \zeta_Q(k; s) \mid 0 \leq h \leq j \leq k, k \in \mathbb{I}_{k-j}, s \in \mathbb{Z}_{\geq 0}^{\text{dep}(k)}, s \leq k \},
\]
where \( (s_1, \ldots, s_d) \leq (k_1, \ldots, k_d) \) means \( s_i \leq k_i \) for all \( 1 \leq i \leq d \). For example, the space \( \mathcal{Z}_2^Q \) is generated by
\[
\zeta_Q(2; 0), \zeta_Q(2; 1), \zeta_Q(2; 2), \zeta_Q(1, 1; 0, 0), \zeta_Q(1, 1; 0, 1), \zeta_Q(1, 1; 1, 0), \zeta_Q(1, 1; 1, 1),
\]
\[
(1-q)\zeta_Q(1; 0), p(1-q)\zeta_Q(1; 0), (1-q)\zeta_Q(1; 1), p(1-q)\zeta_Q(1; 1),
\]
\[
(1-q)^2, p(1-q)^2, p^2(1-q)^2.
\]
As is indicated by the upper \( Q \), \( \mathcal{Z}_k^Q \) is not in \( \mathcal{O} \) (for one, from [BTT18, Remark 2.11] we see that \( \phi_S(\zeta_Q(1, 1; 0, 1)) = \infty \), while \( \phi_A(\zeta_Q(k; s)) = \zeta_Q(k) \) holds for any \( s \in \mathbb{Z}_{\geq 0}^{\text{dep}(k)} \).

Using these objects, we can observe
\[
\zeta_Q(4, 3; 0) - \zeta_Q(3, 1, 1; 2, 1, 0) - \zeta_Q(3, 1, 1; 2, 0, 1) \in (1-q)\mathcal{Z}_1^Q + p(1-q)\mathcal{Z}_1^Q,
\]
from which we can reprove (6.1) for the case \( \mathcal{F} = \mathcal{A} \). Although some of individual terms in the above relation do not converge under the map \( \phi_S \), we can check that main terms in the asymptotic expansion of the above relation are canceled and that the image under the map \( \phi_S \) (modulo \( \pi i \)) coincides with (6.1) for the case \( \mathcal{F} = \mathcal{S} \).

For comparison, we exhibit the numerical dimension of
\[
\tilde{\mathcal{Z}}_k^Q = \mathcal{Z}_k^Q / ((1-q)\mathcal{Z}_k^Q + p(1-q)\mathcal{Z}_k^Q).
\]
Here is a table of dimensions of \( \tilde{\mathcal{Z}}_k^Q \) over \( \mathbb{Q} \) up to weight 5.

\[
\begin{array}{|c|cccccc|}
\hline
k & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
\hline
\text{dim}_Q \mathcal{Z}_k^Q & 0 & 1 & 2 & 6 & 8 & 16 \\
\hline
\end{array}
\]

Remark 6.2. In a similar manner to the proof of Theorem 2.4 (ii), one can show that \( \zeta_Q(k; \{0\}^{\text{dep}(k)}) \) of weight \( k \) lies in \( \mathcal{Z}_k^Q \) (see also [Tas21, Theorem 3.8] with the
case $N = 1$). Since
\[
q^{sm} \equiv q^{(s-1)m} - (1 - q)q^{(s-1)m} \mod \left[ m \right]^k,
\]
we see that elements $\zeta_{\mathbb{Q}}(k; s)$ of weight $k$ with $(\{0\}^{\text{dep}(k)}) \leq s < k$ lies in $Z^O_k$, where $(s_1, \ldots, s_d) < (k_1, \ldots, k_d)$ means $s_i < k_i$ for all $1 \leq i \leq d$.

### 6.3. Relations of $\mathbb{Q}_2$-MZVs.
In this subsection, we give examples of relations among $\zeta_{\mathbb{Q}_2}(k)$’s, which are defined by
\[
\zeta_{\mathbb{Q}_2}(k) = (H_{p-1}(k; q) \mod [p]^2)_p \in \mathbb{Q}_2 \cong \hat{\mathbb{Q}}/[p]^2\hat{\mathbb{Q}}.
\]
As examples of relations, from Proposition 4.6, we obtain
\[
\zeta_{\mathbb{Q}_2}(1) - \frac{p - 1}{2}(1 - q) + \frac{1}{2}[p]_{\mathbb{Q}_2}(2) = 0.
\]
Also, we see from Theorems 5.1 and 5.4 that for each index $k$,
\[
(-1)^{\text{wt}(k)}\zeta_{\mathbb{Q}_2}(k) - \zeta_{\mathbb{Q}_2}(k) - [p] \sum_{l \in \mathbb{Z}_{\geq 0}^{\text{dep}(k)} \text{wt}(l) = 1} b\left( k, l \right) \zeta_{\mathbb{Q}_2}(k + l) = 0,
\]
\[
\zeta^{*}_{\mathbb{Q}_2}(k) + \zeta^{*}_{\mathbb{Q}_2}(k^\vee) + [p] \left( \zeta^{*}_{\mathbb{Q}_2}(1, k) + \zeta^{*}_{\mathbb{Q}_2}(1, k^\vee) - \frac{p + 1}{2}(1 - q)\zeta^{*}_{\mathbb{Q}_2}(k) \right) = 0.
\]
In order to count the number of relations, for $k \geq 1$, let $Z^O_k$ be the $\mathbb{Q}$-vector space spanned by the sets
\[
\{ [p]^h(1 - q)^j \zeta_{\mathbb{Q}_2}(k) \mid 0 \leq h \leq j \leq k, \ k \in \mathbb{I}_{k-j} \}
\]
and
\[
\{ [p][p]^h(1 - q)^j \zeta_{\mathbb{Q}_2}(k) \mid 0 \leq h \leq j \leq k + 1, \ k \in \mathbb{I}_{k+1-j} \}.
\]
For simplicity, we consider
\[
\tilde{Z}^O_k = Z^O_k / ((1 - q)Z^O_k + p(1 - q)Z^O_{k-1}).
\]
The list of numerical dimensions of $\tilde{Z}^O_k$ up to weight 7, which is compared with the dimension of the $\mathbb{Q}$-vector space $\mathbb{Z}^O_k$ spanned by $\zeta_{\mathbb{A}_2}(k) = (H_{p-1}(k) \mod p^2)_p \in \mathbb{A}_2$ of weight $k$ (see [Zha16, p.261]), is as follows.

| $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|-----|---|---|---|---|---|---|---|
| dim$_\mathbb{Q} Z^O_k$ | 0 | 1 | 1 | 2 | 3 | 4 | 7 |
| dim$_\mathbb{Q} Z^O_k$ | 0 | 1 | 1 | 1 | 2 | 2 | 3 |
Appendix A. Proof of Theorem 4.4

In this appendix, we give a proof of Theorem 4.4. Our first goal is to prove

\[ \lim_{m \to \infty} H_{m-1}(k; q_m(t)) = \hat{\xi}(k), \]

from which the equation (4.2) for \( \bullet = \emptyset \) follows, where \( q_m(t) \) was defined to be the solution to (4.1). The equation (4.2) for \( \bullet = \star \) is also obtained from (A.1), together with (2.7) and Proposition A.2, so its proof is omitted. Finally, we prove (4.3) in much the same way. Throughout this section, for simplicity of notations, we write \( \zeta_m = e^{2\pi i/m} \).

A.1. Asymptotic formulas. Note that for each index \( k \), one obtains the power series

\[ H_{m-1}(k; q_m(t)) = \sum_{l \geq 0} \alpha_l(k; m)t^l \in \mathbb{Q}(\zeta_m)[[t]]. \]

Our first task is to give an asymptotic formula for \( \alpha_l(k; m) \) as \( m \to \infty \).

For this, we remark that for each index \( k \) the formula

\[ \alpha_0(k; m) = H_{m-1}(k; \zeta_m) \]

(A.2)

\[ = \sum_{a=0}^{\text{dep}(k)} (-1)^{\text{wt}(k_a)} \zeta^*(k_{\bar{a}}; \gamma_m) \zeta^*(k^a; \gamma_m) + O \left( \frac{\log \gamma_m}{m} \right) \]

is shown in [BTT18, §2.3.2], where \( \gamma_m \) is defined in terms Euler’s constant \( \gamma \) by

\[ \gamma_m = \log \left( \frac{m}{\pi} \right) + \gamma - \frac{\pi i}{2} \]

and \( \gamma_m \) is its complex conjugate. We consider similar asymptotics for \( l \geq 1 \).

Let us begin with a general result on explicit formulas for the coefficients of \( t^l \) \((l \geq 0)\) in the Taylor expansion of \( f(q_m(t)) \) at \( t = 0 \) for any holomorphic function \( f(q) \) at \( q = \zeta_m \).

Proposition A.1. For \( l, j \geq 0 \), we define the rational number \( B_{l,j} \) by

\[ B_{l,j} = \frac{1}{j!} \left. \frac{d^j}{dy^j} \left( \frac{y}{e^y - 1} \right)^l \right|_{y=0} \]

and set

\[ S_{l,j}(m) = \frac{1}{j!} \left. \frac{d^j}{dy^j} (\zeta_m e^{y/m} - 1)^l \right|_{y=0}. \]

(A.3)
Suppose that a function \( f(q) \) is holomorphic in a neighborhood of \( q = \zeta_m \). Set \( f(q_m(t)) = \sum_{l \geq 0} a_l t^l \), where \( a_l \in \mathbb{C} \). Then \( a_0 = f(\zeta_m) \) and, for \( l \geq 1 \), it holds that

\[
a_l = \frac{1}{l} \sum_{j_1+j_2+j_3=l-1 \atop j_1,j_2,j_3 \geq 0} B_{l,j_1} S_{l,j_2}(m) \frac{1}{j_3!m^{j_3+1}} (\theta_q^{j_3+1} f)(\zeta_m),
\]

where \( \theta_q \) is the theta operator

\[
\theta_q = q \frac{d}{dq}.
\]

**Proof.** By definition we have \( a_0 = f(q_m(0)) = f(\zeta_m) \). Suppose that \( l \geq 1 \). Consider the function \( \psi_m(y) = (1 - e^y)/(1 - \zeta_m e^{y/m}) \). Since \( d[m]/dq \) is non-zero at \( q = \zeta_m \), we have \( q_m(\psi_m(y)) = \zeta_m e^{y/m} \). Note that \( \psi_m(0) = 0 \) and \( \psi_m'(0) \neq 0 \). Changing the variable \( t \) to \( y \) by \( t = \psi_m(y) \), we see that

\[
a_l = \text{Res}_{t=0} t^{l-1} f(q_m(t)) \, dt = \text{Res}_{y=0} \psi_m'(y) \psi_m(y)^{-l-1} f(\zeta_m e^{y/m}) \, dy.
\]

The right side is equal to

\[
\text{Res}_{y=0} \left( -\psi_m(y)^{-l}/l \right)' f(\zeta_m e^{y/m}) \, dy = \frac{1}{l} \text{Res}_{y=0} \left\{ \psi_m(y)^{-l} \left( \frac{d}{dy} f(\zeta_m e^{y/m}) \right) \right\} \, dy
\]

Since \( \psi_m(y)^{-l} \) has an \( l \)-th order pole at \( y = 0 \), it is equal to

\[
\frac{1}{l!} \left. \frac{d^{l-1}}{dy^{l-1}} \left\{ y^l \left( \frac{\zeta_m e^{y/m} - 1}{e^y - 1} \right)^l \left( \frac{d}{dy} f(\zeta_m e^{y/m}) \right) \right\} \right|_{y=0} = \frac{1}{l} \sum_{j_1+j_2+j_3=l \atop j_1,j_2,j_3 \geq 0} B_{l,j_1} S_{l,j_2}(m) \frac{1}{j_3!} \left. \frac{d^{j_3+1}}{dy^{j_3+1}} f(\zeta_m e^{y/m}) \right|_{y=0}.
\]

Now the desired formula follows from the relation

\[
\frac{d^k}{dy^k} f(\zeta_m e^{y/m}) = \frac{1}{m^k} (\theta_q^k f)(\zeta_m e^{y/m})
\]

for \( k \geq 0 \). \( \square \)

**Proposition A.2.** Set

(A.4) \hspace{1cm} 1 - q_m(t) = -\frac{2\pi i}{m} \sum_{l \geq 0} \alpha_l(m) t^l,

where \( \alpha_l(m) \in \mathbb{C} \). Then it holds that \( \alpha_0(m) = 1 + O(m^{-1}) \) and \( \alpha_1(m) = O(m^{-1}) \) for \( l \geq 1 \) as \( m \to \infty \).

For the proof, we use the following lemma.
Lemma A.3. For \( l \geq j \geq 0 \), it holds that
\[
S_{l,j}(m) = \frac{1}{m!} \binom{l}{j} (2\pi i)^{l-j} (1 + O(m^{-1})) \quad (m \to \infty).
\]

Proof. Substituting \( q = \zeta_m e^{y/m} \) into (A.3), we have
\[
S_{l,j}(m) = \frac{1}{j!} \frac{\theta_j}{m^j} (q - 1)^l|_{q=\zeta_m}.
\]
It holds that
\[
\theta_j = \sum_{n=1}^{j} \{ \frac{j}{n} \} q^n \frac{d^n}{dq^n},
\]
where \( \{ \frac{j}{n} \} \) is the Stirling number of the second kind defined by
\[
\{ \frac{j}{0} \} = \delta_{j,0}, \quad \{ \frac{j+1}{n} \} = \{ \frac{j}{n-1} \} + n \{ \frac{j}{n} \}.
\]
Note that \( \{ \frac{j}{j} \} = 1 \). Therefore
\[
S_{l,j}(m) = \frac{1}{j! m^j} \sum_{n=1}^{j} \{ \frac{j}{n} \} q^n \frac{d^n}{dq^n} (q - 1)^l|_{q=\zeta_m}
\]
\[
= \frac{1}{j! m^j} \sum_{n=1}^{j} \{ \frac{k}{n} \} q^n (l-1) \cdots (l-n+1)(q-1)^{l-n}|_{q=\zeta_m}
\]
\[
= \frac{1}{j! m^j} \sum_{n=1}^{j} n! \{ \frac{j}{n} \} \binom{l}{n} \zeta_m^n (\zeta_m - 1)^{l-n}.
\]
Since \( \zeta_m = 1 + \frac{2\pi i}{m} + O(m^{-2}) \) as \( m \to \infty \) and the coefficient of \( \zeta_m^n (\zeta_m - 1)^{l-n} \) in the above does not depend on \( m \), we have
\[
= \frac{1}{j! m^j} \sum_{n=1}^{j} n! \{ \frac{j}{n} \} \binom{l}{n} \left( \frac{2\pi i}{m} \right)^{l-n} (1 + O(m^{-1}))
\]
\[
= \frac{1}{m^j} \binom{l}{j} \left( \frac{2\pi i}{m} \right)^{l-j} (1 + O(m^{-1}))
\]
from which the statement follows. \( \square \)

Proof of Proposition A.2. Setting \( t = 0 \) in (A.4), we obtain \( 1 - \zeta_m = -\frac{2\pi i}{m} \alpha_0(m) \). Hence \( \alpha_0(m) = 1 + O(m^{-1}) \). For \( l \geq 1 \), applying Proposition A.1 to the case \( f(q) = 1 - q \), we see that
\[
-\frac{2\pi i}{m} \alpha_l(m) = \frac{1}{l} \sum_{j_1+j_2=l-1 \atop j_1,j_2 \geq 0} B_{l,j_1,j_2}(m) \frac{-\zeta_m}{m}.
\]
The above expression and Lemma A.3 imply $\alpha_l(m) = O(m^{-l})$. □

Remark A.4. In this paper, we only use the asymptotic formula for $q_m(t)$ described in Proposition A.2. However, using the standard technique, one can compute the Taylor expansion of $q_m(t)$ at $t = 0$. It is given by

$$
q_m(t) = \zeta_m \sum_{l \geq 0} t^l \sum_{j=0}^l \frac{(-\zeta_m)^j}{(j+1)!} \left( \frac{j+1}{m} \right)_l,
$$

where $(a)_l = a(a+1) \cdots (a+l-1)$.

For an index $k = (k_1, \ldots, k_d)$ and a positive integer $m$, we set

$$
\tilde{H}_{m-1}(k; q) = \left( -\frac{m}{2\pi i} (1 - q) \right)^{-\text{wt}(k)} H_{m-1}(k; q)
$$

and write

$$
\tilde{H}_{m-1}(k; q_m(t)) = \sum_{l=0}^{\infty} \tilde{\alpha}_l(k; m) t^l.
$$

Proposition A.2 implies that

(A.5) \quad $H_{m-1}(k; q_m(t)) = \tilde{H}_{m-1}(k; q_m(t)) \left( 1 + \sum_{l \geq 0} O(m^{-1}) t^l \right).$

Thus, we have

$$
\alpha_0(k; m) = \tilde{\alpha}_0(k; m) \left( 1 + O(m^{-1}) \right) \quad (m \to \infty)
$$

and (A.2) gives the asymptotic for $\tilde{\alpha}_0(k; m)$. It also follows from (A.5) that, if the limit $\lim_{m \to \infty} \tilde{\alpha}_l(k; m)$ exists, we get

(A.6) \quad $\lim_{n \to \infty} \tilde{\alpha}_l(k; m) = \lim_{n \to \infty} \alpha_l(k; m)$. 
Now consider the asymptotics of $\tilde{\alpha}_l(k; m)$ for $l \geq 1$. Using Proposition A.1 and then Lemma A.3, we see that

\begin{equation}
(A.7)
\tilde{\alpha}_l(k; m) = \frac{1}{l} \sum_{j_1, j_2, j_3 = l-1} B_{l, j_1} S_{l, j_2} (m) \frac{1}{j_2! m^{j_2+1}} (q^{j_2+1} H_{m-1})(k; \zeta_m)
\end{equation}

\[= \frac{1}{l} \sum_{j_1, j_2, j_3 = l-1} B_{l, j_1} \frac{1}{m^l} \binom{l}{j_2} (2\pi i)^{l-j_2} (1 + O(m^{-1})) \]

\[\times \frac{j_3 + 1}{m^{j_3+1}} \sum_{l_1, \ldots, l_d = l-1} \sum_{l_1, \ldots, l_d \geq 0} \prod_{a=1}^d \left( -\frac{2\pi i}{m} \right)^{k_a} \frac{1}{l_a!} \frac{q^{(k_a-1)m a}}{(1 - q^{m a})^{k_a}} \bigg|_{q=\zeta_m}.
\]

Lemma A.5. For $l \geq 0$ and $k, m \geq 1$, it holds that

\[\frac{1}{l!} \frac{q^l}{q} \frac{q^{(k-1)m}}{(1-q^m)^k} = m^l \sum_{s=0}^l T_{s,l}(k) \binom{s+k-1}{s}(1-q^{m})^{k+s},\]

where

\[ T_{s,l}(k) = \frac{s!}{l!} \sum_{a=s}^l \binom{l}{a} \binom{a}{s} (k-1)^{l-a}.\]

Proof. We may assume that $|q| < 1$. We calculate the generating function:

\[\sum_{l \geq 0} \frac{X^l}{l!} \frac{q^{(k-1)m}}{(1-q^m)^k} = \sum_{l, j \geq 0} \frac{X^l}{l!} \binom{k+j-1}{j} q^l q^{(k+j-1)m}\]

\[= \sum_{l, j \geq 0} \frac{((k+j-1)mX)^l}{l!} \binom{k+j-1}{j} q^{(k+j-1)m}\]

\[= \sum_{j \geq 0} \frac{(k+j-1)mX}{j!} q^{(k+j-1)m} e^{(k+j-1)mX} = e^{(k-1)mX} \frac{q^{(k-1)m}}{(1-q^m e^{mX})^k}.
\]

Now compute

\[\frac{q^{(k-1)m}}{(1-q^m e^{mX})^k} = \frac{q^{(k-1)m}}{(1-q^m)^k} \left( 1 - \frac{q^m}{1-q^m} (e^{mX} - 1) \right)^{-k}\]

\[= \sum_{s=0}^\infty \binom{k+s-1}{s} \frac{q^{(k+s-1)m}}{(1-q^m)^{k+s}} (e^{mX} - 1)^s\]

\[= \sum_{s=0}^\infty \binom{k+s-1}{s} \frac{q^{(k+s-1)m}}{(1-q^m)^{k+s}} \sum_{j=s}^\infty \binom{j}{s} \frac{s!}{j!} (mX)^j.
\]
where for the third equality we have used [AIK, Eq.(7)]. Thus, we obtain
\[
\frac{1}{l!} \theta_q^{(l)} \frac{q^{(k-1)m}}{(1 - q^m)^k} = \sum_{j_1, j_2 \geq 0} \left( \frac{(k-1)m}{j_1!} \right) \sum_{j = 0}^{j_2} \left( k + s - 1 \right) \frac{q^{(k+s-1)m}}{(1 - q^m)^{k + s}} \left( \frac{j_2}{j} \right) s!
\]

which is the desired formula.

Applying Lemma A.5 to (A.7), we see that
\[
(A.8) \quad \tilde{\alpha}_l(k; m) = \sum_{j_1, j_2 \geq 0} \frac{l-j_1-j_2}{l} B_{t,j_1} \frac{1}{m^l} \left( \frac{l}{j_2} \right) (2\pi i)^{l-j_2} (1 + O(m^{-1}))
\]
\[\times \sum_{s=(s_1, \ldots, s_d) \in \mathbb{Z}_{\geq 0}^d \atop l_i \geq s_i \geq 0 \atop 1 \leq i \leq d \atop s_d \geq 0} (-m) \text{wt}(s) \left\{ \prod_{a=1}^{d} \left( k_a + s_a - 1 \right) T_{s_a, l_a}(k_a) \right\} Z_{m-1}(l; k + s),
\]
where $Z_{m-1}(l; k)$ is defined by
\[
(A.9) \quad Z_{m-1}(l; k) = \sum_{m-1 \geq m_1 > \ldots > m_d > 0} \prod_{a=1}^{d} \left( \frac{m_a}{m} \right) \left( \frac{2\pi i}{m} \right)^{k_a} \frac{\zeta_m^{(k_a-1)m_a}}{1 - \zeta_m^{m_a k_a}}
\]
for $l = (l_1, \ldots, l_d) \in \mathbb{Z}_{\geq 0}^d$ and $k = (k_1, \ldots, k_d) \in \mathbb{Z}_{\geq 1}^d$.

**Lemma A.6.** For $l \in \mathbb{Z}_{\geq 0}^d$ and an index $k \in \mathbb{Z}_{\geq 1}^d$, we have $Z_{m-1}(l; k) = O((\log m)^d)$ as $m \to \infty$.

**Proof.** We see that
\[
(A.10) \quad |Z_{m-1}(l; k)| \leq \sum_{m-1 \geq m_1 > \ldots > m_d > 0} \prod_{a=1}^{d} \left| \left( \frac{2\pi i}{m} \right)^{k_a} \frac{\zeta_m^{(k_a-1)m_a}}{1 - \zeta_m^{m_a k_a}} \right|.
\]
For an index \( k = (k_1, \ldots, k_d) \) define
\[
\tilde{Z}_m(k) = \sum_{m/2 \geq m_1 > \cdots > m_d > 0} \prod_{a=1}^d \left| \left( \frac{-2\pi i}{m} \right)^{k_a} \frac{\zeta_m^{(k_a-1)m_a}}{(1 - \zeta_m^{m_a})^{k_a}} \right|.
\]

By a similar argument to [BTT18, §2.3.2], the right side of (A.10) is bounded from above by \( \sum_{a=0}^d \tilde{Z}_m(k_a) \tilde{Z}_m(k^a) \). Hence it suffices to show that \( \tilde{Z}_m(k) = O((\log m)^d) \) for \( k \in \mathbb{Z}^d_{\geq 1} \).

For \( k \geq 1 \), we define the function \( \varphi_k(x) \) by
\[
\varphi_k(x) = (-\pi i x)^k \frac{e^{(k-1)x}}{(1 - e^{\pi i x})^k}.
\]
Then
\[
\tilde{Z}_m(k) = \sum_{m/2 \geq m_1 > \cdots > m_d > 0} \prod_{a=1}^d |m_a^{-k_a} \varphi_k(2m_a/m)|.
\]
Since \( \varphi_k(x) \) is bounded in the unit disc \( |x| \leq 1 \), there exists a positive constant \( C_k \) such that
\[
\tilde{Z}_m(k) \leq C_k \sum_{m/2 \geq m_1 > \cdots > m_d > 0} \prod_{a=1}^d m_a^{-k_a}.
\]
Hence \( \tilde{Z}_m(k) = O((\log m)^d) \) because \( k \in \mathbb{Z}^d_{\geq 1} \). \( \square \)

Lemma A.6 implies that the summand of (A.8) is \( O((\log m)^J/m) \) for some \( J \geq 1 \) unless \( \text{wt}(s) = l \), in which case \( s = l \) and \( j_1 = j_2 = 0 \). Since \( B_{l,0} = 1 \), for an index \( k \) we have
\[
\tilde{\alpha}_l(k, m) = (-1)^l \sum_{l \in \mathbb{Z}^d_{\geq 1}} b \left( \frac{k}{l} \right) Z_{m-1}(l; k + l) + O((\log m)^{J_{k,l}}/m)
\]
for some \( J_{k,l} \geq 1 \), where we have used the notation in (1.3).

For \( l = (l_1, \ldots, l_d) \in \mathbb{Z}^d_{\geq 0} \) and \( k = (k_1, \ldots, k_d) \in \mathbb{Z}^d_{\geq 1} \), we set
\[
A_m^- (l; k) = \sum_{m/2 > m_1 > \cdots > m_d > 0} \prod_{a=1}^d \left( \frac{m_a}{m} \right)^{l_a} \left( -\frac{2\pi i}{m} \right)^{k_a} \frac{\zeta_m^{(k_a-1)m_a}}{(1 - \zeta_m^{m_a})^{k_a}}
\]
and define \( A_m^+(l; k) \) by (A.13) where the range of summation \( m/2 > m_1 > \cdots > m_d > 0 \) is replaced by \( m/2 \geq m_1 > \cdots > m_d > 0 \). We set \( A_m^+(\emptyset; \emptyset) = 1 \). Then it
holds that
\[
Z_{m-1}(l; k + l) = \sum_{a=0}^{d} \left\{ \sum_{l_j \geq s_j \geq 0} \left( \prod_{1 \leq j \leq a} (-1)^{l_j + l_j + s_j} \binom{l_j}{s_j} \right) \overline{A_{m}^{+}(s_a, \ldots, s_1; k_a + l_a)} \right\} \times A_{m}^{-}(l^a; k^a + l^a),
\]
where the bar on $A_{m}^{+}$ means the complex conjugate.

**Lemma A.7.** Let $s \in \mathbb{Z}_{\geq 0}^d$ and $k \in \mathbb{Z}_{\geq 1}^d$. Suppose that $d \geq 1$ and $k_a - 1 \geq s_a \geq 0$ for $1 \leq a \leq r$. If $s \neq (0, \ldots, 0)$, it holds that $A_{m}^{\pm}(s; k) = O((\log m)^{d}/m)$. If $s = (0, \ldots, 0)$, we have
\[
A_{m}^{\pm}(\{0\}^d; k) = \zeta^*(k; \gamma_{m}) + O((\log m)^{J_k}/m)
\]
for some $J_k \geq 1$.

**Proof.** Since $A_{m}^{+}(s; k) = A_{m}^{-}(s; k)$ if $m$ is odd and
\[
A_{m}^{+}(s; k) = -\frac{1}{2^{s_1}} \left( \frac{\pi i}{m} \right)^{k_1} A_{m}^{-}(s^1; k^1) + A_{m}^{-}(s; k)
\]
if $m$ is even, it suffices to show the statement for $A_{m}^{-}(s; k)$. For $s = (0, \ldots, 0)$ it is proved in [BTT18, Proposition 2.9]. Using the function $\varphi_k(x)$ defined by (A.11), we rewrite as
\[
A_{m}^{-}(s; k) = m^{-\text{wt}(s)} \sum_{m/2 > m_1 > \cdots > m_d > 0} \prod_{a=1}^{d} \frac{\varphi_{k_a}(2m_a/m)}{m_{k_a - s_a}}.
\]
By the same argument as in the proof of Lemma A.6, we see that the sum in the right side is $O((\log m)^d)$. Hence, if $\text{wt}(s) \geq 1$, it holds $A_{m}^{-}(s; k) = O((\log m)^d/m)$. \qed

**Theorem A.8.** For all $l \geq 1$ and each index $k$ of depth $d$, we have
(A.14)
\[
\tilde{\alpha}_l(k; m) = \sum_{a=1}^{d} (-1)^{\text{wt}(k_a)} \sum_{l \in \mathbb{N}_{>0}} b\left( \binom{k_a}{l} \right) \zeta^*(k_a + l, \gamma_{m}) \zeta^*(k^a; \gamma_{m}) + O\left( \frac{(\log m)^{J_{k,l}}}{m} \right)
\]
for some integer $J_{k,l} \geq 1$.

**Proof.** Applying Lemma A.7 to (A.12), we obtain the desired result. \qed

A.2. **Proof of** (A.1). In order to check that the limit $\lim_{m \to \infty} (H_{m-1}(k; q_{m}(t))$ exists, we need the following lemma, from which, by Theorem A.8, (A.1) follows.
Lemma A.9. For any index $k$, the sum
\[
\sum_{a=0}^{\text{dep}(k)} (-1)^{\text{wt}(ka)} \sum_{l \in \mathbb{Z}_{\geq 0}^{\text{dep}(a)}} t^{\text{wt}(t)} b\left(\frac{ka}{l}\right) \zeta^* \left(\frac{ka + l}{2} + T + \frac{\pi i}{2}\right). \zeta^* \left(\frac{ka}{2} - \frac{\pi i}{2}\right).
\]
does not depend on $T$ and coincides with $\hat{\xi}(k) \in \mathcal{Z}[\pi i][[t]]$.

Our proof of Lemma A.9 is done by a similar computation with [Hir20, Jar2]. We repeat it for convenience.

Recall the notation from §2.1. Consider the algebraic projection
\[
\text{reg}_0 : h_{\omega} \rightarrow h_{\omega}^1
\]
which sends $x_0$ to 0. It is well-known that
\[
\text{reg}_0(x_k x_0^l) = (-1)^l \sum_{l \in \mathbb{Z}_{\geq 0}^{\text{dep}(a)}} b\left(\frac{k}{l}\right) x_{k+l}, \tag{A.15}
\]
holds for any index $k$ of depth $d$ and $l \geq 0$ (see e.g., [Bro12, p.955]). Denote by $\{x_0, x_1\}^{\times}$ the set of words consisting of $x_0$ and $x_1$. We assume that the set $\{x_0, x_1\}^{\times}$ contains the empty word $\emptyset$. Let us consider the two non-commutative generating series
\[
\Phi_{\omega}(T) = \sum_{w \in \{x_0, x_1\}^{\times}} Z_{\omega}(\text{reg}_0(w)) w \quad \text{and} \quad \Phi^*(T) = \Lambda(x_1) \Phi_{\omega}(T),
\]
which lie in $\mathbb{R}[T] \langle \langle x_0, x_1 \rangle \rangle$, where we set $Z_{\omega}(\emptyset) = 1$ and
\[
\Lambda(x) = \exp \left( \sum_{n \geq 2} \frac{(-1)^{n-1}}{n} \zeta(n) x^n \right).
\]

For a non-commutative power series $S \in \mathbb{R}[T] \langle \langle x_0, x_1 \rangle \rangle$, we denote by $S[w]$ the coefficient of a word $w$ in $S$.

Lemma A.10. [Jar2, Proposition 3.2.2] For each index $k$ and $l \geq 0$ we have
\[
\Phi^*(T)[x_k x_0^l] = (-1)^l \sum_{l \in \mathbb{Z}_{\geq 0}^{\text{dep}(k)}} b\left(\frac{k}{l}\right) \zeta^* (k + l; T). \tag{A.16}
\]

Proof. Denote by $\{y_k \mid k \geq 1\}^{\times}$ the set of words consisting of $y_k$ ($k \geq 1$). Let
\[
\Psi^*(T) = \sum_{w \in \{y_k \mid k \geq 1\}^{\times}} Z^*(w) w,
\]
where we set $Z^*(\emptyset) = 1$. Define the $\mathbb{R}[T]$-linear map

$$\pi_Y : \mathbb{R}[T][\langle x_0, x_1 \rangle] \rightarrow \mathbb{R}[T][\langle y_k \mid k \geq 1 \rangle]$$

by $\pi_Y(x_k) = y_k$ for $k \in \mathbb{Z}_{d_1}^d (d \geq 0)$ and $\pi_Y(wx_0) = 0$ for $w \in \mathcal{H}$. Then the regularization theorem by Racinet [Rac02] (see also [IKZ06]) states the equality

(A.17) $$\Psi^*(T) = \pi_Y(\Lambda(x_1)\Phi^\mu(T)).$$

This shows that

(A.18) $$\Phi^*(T)[x_k] = \Lambda(x_1)\Phi^\mu(T)[x_k] = \Psi^*(T)[y_k]$$

holds for any index $k$.

Let $l \geq 1$. For an admissible index $k$, by using (A.15) and (A.18), we see

$$\Phi^*(T)[x_k^l] = \Lambda(x_1)\Phi^\mu(T)[x_k^l] = \Phi^\mu(T)[x_k^l] = (-1)^l \sum_{l \in \mathbb{Z}_{d_1}^d(k) \atop wt(l) = l} b \binom{k}{l} \Phi^\mu(T)[x_k^l] = (-1)^l \sum_{l \in \mathbb{Z}_{d_1}^d(k) \atop wt(l) = l} b \binom{k}{l} \Psi^*(T)[y_k^l],$$

from which (A.16) follows.

Let us consider the case $k = (1, \ldots, 1, k_{a+1}, \ldots, k_d)$ with $k_{a+1} \geq 2$ and $a \geq 1$. Set

$$\Lambda(x) = \sum_{j \geq 0} \lambda_j x^j.$$ Using (A.15), one computes

$$\Phi^*(T)[x_k^l] = \sum_{j=0}^a \lambda_j \Phi^\mu(T)[x_k^l] = \sum_{j=0}^a \lambda_j (-1)^l \sum_{l \in \mathbb{Z}_{d_1}^d(k) \atop wt(l) = l} b \binom{k}{l} \Phi^\mu(T)[x_k^l]$$

$$= (-1)^l \sum_{j=0}^a \lambda_j \sum_{l = (l_1, \ldots, l_d) \in \mathbb{Z}_{d_1}^d \atop wt(l) = l \atop l_1 = \ldots = l_j = 0} b \binom{k}{l} \Phi^\mu(T)[x_k^l].$$

For $0 \leq s \leq a$ we set

$$I_s = \{l \in \mathbb{Z}_{d_1}^d \mid wt(l) = l, l_1 = \ldots = l_s = 0\}, \quad I_s^+ = \{l \in I_s \mid l_{s+1} \geq 1\}.$$ From the above calculation, we see that

$$(-1)^l \Phi^*(T)[x_k^l] = \sum_{j=0}^a \lambda_j \sum_{l \in I_s} b \binom{k}{l} \Phi^\mu(T)[x_k^l].$$
Using \( I_j = I_j^+ \sqcup \cdots \sqcup I_{a-1}^+ \sqcup I_a \), we decompose the right side into the two parts

\[
R_1 = \sum_{j=0}^{a-1} \sum_{s=j}^{a-1} L_j \sum_{l \in I_s^+} b(k_l) \Phi^w(T)[x_{k_j+l}],
\]

\[
R_2 = \sum_{j=0}^{a} L_j \sum_{l \in I_a} b(k_l) \Phi^w(T)[x_{k_j+l}].
\]

For \( j \leq s \leq a-1 \) and \( l \in I_s^+ \) we have

\[
b(k_l) = b(k_s^l), \quad x_{k_j+l} = x_1^{s-j} x_{k_s^l+l^s}
\]

and \( k^s + l^s \) is admissible. Hence

\[
R_1 = \sum_{s=0}^{a-1} \sum_{l \in I_s^+} b(k_s^l) \sum_{j=0}^{s} \Phi^w(T)[x_1^{s-j} x_{k_s^l+l^s}]
\]

\[
= \sum_{s=0}^{a-1} \sum_{l \in I_s^+} b(k_s^l) \Phi^w(T)[x_1^{s} x_{k_s^l+l^s}] = \sum_{s=0}^{a-1} \sum_{l \in I_s^+} b(k_l) \Phi^w(T)[x_{k+l}].
\]

Similarly we see that

\[
R_2 = \sum_{l \in I_a} b(k_l) \Phi^w(T)[x_{k+l}].
\]

Since the direct sum \( I_0^+ \sqcup \cdots \sqcup I_{a-1}^+ \sqcup I_a \) is equal to the set of \( l \in \mathbb{Z}_d^+ \) with \( \text{wt}(l) = l \), we find that

\[
R_1 + R_2 = \sum_{l \in \mathbb{Z}_d^+} b(k_l) \Phi^w(T)[x_{k+l}] = \sum_{l \in \mathbb{Z}_d^+} b(k_l) \Phi^w(T)[y_{k+l}].
\]

This completes the proof. \( \square \)

Define the \( \mathbb{R}[T] \)-linear map \( \sigma : \mathbb{R}[T] \langle \langle x_0, x_1 \rangle \rangle \to \mathbb{R}[T] \langle \langle x_0, x_1 \rangle \rangle \) by

\[
\sigma(x_{a_1} \cdots x_{a_k}) = (-1)^k x_{a_k} \cdots x_{a_1}.
\]

This gives the antipode of the shuffle coalgebra \( \mathbb{R}[T] \langle \langle x_0, x_1 \rangle \rangle \). Thus, for any algebra homomorphism \( \varphi : \mathfrak{h}_w \to \mathbb{R}[T] \), its non-commutative generating series \( S = \sum_w \varphi(w)w \) is group-like with respect to the shuffle coproduct and satisfies \( \sigma(S)S = 1 \). We let

\[
\Xi(T_1, T_2) = \sigma(\Phi^w(T_1)) x_1 \Phi^w(T_2).
\]
Proposition A.11. For any index $k$ and $l \geq 1$, we have
\[
\Xi(T_1, T_2)[x_0^l x_1 x_k] = \sum_{a=0}^{\text{dep}(k)} (-1)^{\text{wt}(ka)} \sum_{l \in \mathbb{N}_0, \text{wt}(l)=l} b\left(\frac{ka}{l}\right) \zeta^*(\frac{k_a+T_1}{l}; T_1) \zeta^*(k^a; T_2)
\]

Proof. Let $k = (k_1, \ldots, k_a)$. One computes
\[
\Xi(T_1, T_2)[x_0^l x_1 x_k] = \sum_{a=0}^{\text{dep}(k)} \sigma\left(\Phi^*(T_1)\right)[x_0^l x_1 x_0^{-1} \cdots x_1 x_0^{-1}][x_k^a] \Phi^*(T_2)[x_k^a]
\]
\[
= \sum_{a=1}^{\text{dep}(k)} (-1)^{l+\text{wt}(ka)} \Phi^*(T_1)[x_0^{-1} x_1 \cdots x_0^{-1} x_0^l] \Phi^*(T_2)[x_k^a].
\]
Thus, the desired formula follows from Lemma A.10.

Proposition A.12. [Hir20, Theorem 9] Let $\Phi_{\exp}(T) = \sigma(\Phi^{\mu}(0)) \exp(T x_1) \Phi^{\mu}(0)$. Then we have
\[
\Xi(T_1, T_2) = \frac{1}{2\pi i} \left(\Phi_{\exp}(\pi i + T_2 - T_1) - \Phi_{\exp}(-\pi i + T_2 - T_1)\right).
\]
In particular, it holds that
\[
\Xi(T + \frac{\pi i}{2}, T - \frac{\pi i}{2}) = \frac{1}{2\pi i} \left(\Phi_{\exp}(0) - \Phi_{\exp}(-2\pi i)\right),
\]
which is independent of $T$.

Proof. Since $\Phi^{\mu}(T) = \exp(T x_1) \Phi^{\mu}(0)$, one computes
\[
\Xi(T_1, T_2) = \sigma(\Lambda(x_1) \Phi^{\mu}(T_1)) \Lambda(x_1) \Phi^{\mu}(T_2)
\]
\[
= \sigma\left(\Phi^{\mu}(T_1)\right)\Lambda(-x_1) \Lambda(x_1) \Phi^{\mu}(T_2)
\]
\[
= \sigma\left(\Phi^{\mu}(0)\right) \exp(-T_1 x_1) \Lambda(-x_1) \Lambda(x_1) \exp(T_2 x_1) \Phi^{\mu}(0)
\]
\[
= \sigma\left(\Phi^{\mu}(0)\right) \frac{\sin \pi x_1}{\pi} \exp((T_2 - T_1) x_1) \Phi^{\mu}(0)
\]
\[
= \sigma\left(\Phi^{\mu}(0)\right) \left(\exp((-\pi i + T_2 - T_1)x_1) - \exp((-\pi i + T_2 - T_1)x_1)\right) \Phi^{\mu}(0),
\]
from which the statement follows.

Proof of Lemma A.9. Lemma A.9 follows from Propositions A.11 and A.12.

A.3. Proof of (4.3). We turn to the proof of (4.3). Define $\beta_l(k; m) \in \mathbb{C}$ ($l \geq 0, m \geq 1$) by
\[
\left(-\frac{m}{2\pi t} (1 - q_m(t))\right)^{-\text{wt}(k)} H_{m-1}(k; q_m(t)) = \sum_{l \geq 0} \beta_l(k; m) t^l.
\]
We show the limit of $\beta_l(k; m)$ as $m \to +\infty$ converges. Then we have

$$\phi_S(\zeta_S(k)) = \sum_{l \geq 0} (\lim_{m \to \infty} \beta_l(k; m)) t^l.$$

Using the equality

$$\frac{1}{l!} \frac{q^m}{(1 - q^m)^k} = m^l \sum_{s=0}^{l} (-1)^{s+l} T_{s,l}(k) \left( \frac{s+k-1}{s} \right) \frac{q^m}{(1 - q^m)^{k+s}}$$

for $l \geq 0$ and $k, m \geq 1$, which is shown by the same way as Lemma A.5, we see that

$$\beta_l(k; m) = \sum_{j_1, j_2 \geq 0 \atop l = (l_1, \ldots, l_d) \in \mathbb{Z}_{\geq 0}^{d}} \frac{l - j_1 - j_2}{l} B_{l, j_1} \frac{1}{m^l} \left( \frac{l}{j_2} \right) (2\pi i)^{l-j_2} (1 + O(m^{-1}))$$

$$\times \sum_{s=(s_1, \ldots, s_d) \in \mathbb{Z}_{\geq 0}^{d} \atop l_a \geq s_a \geq 0 \atop (1 \leq a \leq d)} \left( -\frac{m}{2\pi i} \right)^{wt(s)} (-1)^{wt(s)+wt(t)} b \left( \frac{k}{s} \right) \prod_{a=1}^{d} T_{s_a, l_a}(k_a) Z_{m-1}(l; k + s),$$

where $Z_{m-1}(l; k)$ is the complex number defined by (A.9). Now the desired equality is obtained from the above expression in a similar manner to the proof of (4.2).

For the star version, we use

$$\frac{q^m}{[m]^{k_1} [m]^{k_2}} = \frac{q^m}{[m]^{k_1+k_2}} + (q - 1) \frac{q^m}{[m]^{k_1+k_2-1}}$$

to obtain the relations of the following form for any index $k = (k_1, \ldots, k_d)$:

$$\Pi_m(k; q) = \Pi_m(l; q) + \sum_{wt(k') < wt(k)} (q - 1)^{wt(k)-wt(k')} c_{k,k'} \Pi_m(k'; q),$$

where the sum $\sum_l$ is over all indices $l$ of the form $(k_1 \square k_2 \square \cdots \square k_d)$ in which $\square$ is either ’+’ (plus) or ’,’ (comma), and $c_{k,k'}$ is an integer independent on $m$. Then the result is a consequence of the limit formula $\lim_{m \to \infty} \Pi_m(k; q_m(t)) = \hat{\xi}(k)$ and the definition of $\hat{\xi}^*(k)$. So we are done.

**APPENDIX B. PROOFS OF RELATIONS**

**B.1. PROOF OF REVERSAL FORMULAS.**

**Lemma B.1.** Suppose that $p$ is a prime, $p > m \geq 1$ and $k \geq 1$. It holds that

$$\frac{1}{[p-m]^k} = \left( -(q^p)^{-1} \frac{q^m}{[m]} \right)^k \sum_{l=0}^{n-1} \binom{k+l-1}{l} \left( (q^p)^{-1} \frac{q^m}{[m]} \right)^l$$


in $\mathbb{Z}_{p,n}$ for all $n \geq 1$.

Proof. Note that there exists $f_{k,n}(x) \in \mathbb{Z}[x]$ such that

$$(1 - x)^k \sum_{l=0}^{n-1} \binom{k + l - 1}{l} x^l = 1 + x^nf_{k,n}(x).$$

Set $x = (q^p)^{-1}[p]q^m/[m]$ and use

$$1 - (q^p)^{-1}[p]q^m/m] = (q^p)^{-1}q^m/[m] (q^{p-m}[m] - [p]) = -(q^p)^{-1}q^m/[m] [p - m].$$

Then we obtain (B.1). □

Proof of Theorem 5.1. It suffices to show the identity

$$H_{p-1}(k; q) = \left((q^p)^{-1} q^{\deg(k)}\right) \sum_{l \in \mathbb{Z}^\geq 0 \cap wt(l) < n} \binom{k}{l} \left((q^p)^{-1} [p]\right)^{wt(l)} \left(H_{p-1}(k + l; q)\right).$$

in $\mathbb{Z}_{p,n}$ for $\bullet \in \{\emptyset, \ast\}$, any prime $p$ and $n \geq 1$. It is obtained by changing the summation variable $m_a$ to $p - m_a$ in $H_{p-1}(k; q)$ and using (B.1). □

Proof of Corollary 5.2. Since $\phi_F(q^p) = 1$, applying Theorems 4.3 and 4.4 to Theorem 5.1, we get the desired formulas. □

B.2. Proof of duality formulas.

Proof of Theorem 5.4. Set $k = (k_1, \ldots, k_d)$ and $k' = (k'_1, \ldots, k'_s)$. We start from a $q$-analogue of the duality formula due to Bradley [Bra05-2] (see also [Kaw10]):

$$\sum_{n \geq m_1 \geq \cdots \geq m_d > 0} (-1)^{m_1-1} q^{m_1(m_1-1)/2} \prod_{a=1}^{d} \frac{q^{(ka-1)m_a}}{[m_a]^{ka}}$$

$$= \sum_{n=m_1 \geq m_2 \geq \cdots \geq m_s > 0} \frac{1}{[m_1]^{k_1} \prod_{a=2}^{s} \frac{q^{m_a}}{[m_a]^{k_a}}}.$$

where $\binom{n}{m}$ is the $q$-binomial coefficient

$$\binom{n}{m} = \prod_{j=1}^{m} \frac{n - (j - 1)}{[j]}.$$

Multiply the both sides by $(-1)^n q^{(p-n)(p-n-1)/2} \left[p^{-1}\right]$ and take the sum over $1 \leq n \leq p - 1$ using the equalities

$$\binom{p-1}{n-1} \binom{n-1}{m_1-1} = \binom{p-1}{m_1-1} \binom{p-1}{n-m_1}. $$
and
\[ \sum_{n=m_1}^{p-1} (-1)^{p-n} q^{n(n-1)/2} \binom{p-m_1}{n-m_1} = (-1)^{p-1}. \]

Then we obtain
\[ (-1)^{p-1} \sum_{p>m_1 \geq \cdots \geq m_d > 0} (-1)^{m_1-1} q^{m_1(m_1-1)/2} \sum_{p>m_1 \geq \cdots \geq m_d > 0} \frac{q^{(k_{a-1})m_a}}{[m_a]^{k_a}} \]
\[ \quad = \sum_{p>m_1 \geq \cdots \geq m_s > 0} (-1)^{m_1} q^{(p-m_1)(p-m_1-1)/2} \binom{p}{m_1-1} \frac{1}{[m_1]^{k_1'}} \prod_{a=2}^{s} \frac{q^{m_a}}{[m_a]^{k_a'}}. \]

It is an identity of rational functions in \( q \). Using Proposition B.1, we see that the following equalities hold in \( \mathbb{Z}_{p,n} \) for any \( n \geq 1 \):
\[ (-1)^{m-1} q^{m(m-1)/2} \binom{p}{m-1} = (-1)^{p-1} q^{p(p-1)/2} \prod_{a=m}^{p-1} \frac{[a]}{[a] - [p]} \]
\[ = (-1)^{p-1} q^{p(p-1)/2} \left( 1 + \sum_{l=1}^{n-1} [p]^l \sum_{p>m_1 \geq \cdots \geq m_j > 0} \prod_{j=1}^{l} \frac{1}{[m_j]} \right) \]
and
\[ (-1)^{m} q^{(p-m)(p-m-1)/2} \binom{p}{m-1} = (-1)^{m} q^{(p-m)(p-m-1)/2} \prod_{a=m}^{p-1} \frac{[a]}{p-a} \]
\[ = (-1)^p (q^p - 1)^m q \left( 1 + \sum_{l=1}^{n-1} ((q^p - 1)^l[p])^l \sum_{p>m_1 \geq \cdots \geq m_j > 0} \prod_{j=1}^{l} \frac{q^{m_j}}{[m_j]} \right). \]

Hence for any prime \( p \) we obtain
\[ (-1)^{p-1} q^{p(p+1)/2} \sum_{l=0}^{n-1} [p]^l H^*_{p-1}({\{1\}}^l, k; q) = -\sum_{l=0}^{n-1} (q^{-p}[p])^l H^*_{p-1}({\{1\}}^l, k^\vee; q) \mod [p]^n, \]
which completes the proof. \(\square\)

**Proof of Corollary 5.5.** The relation (5.1) for \( \mathcal{F} = \mathcal{A} \) is obtained by applying \( \phi_\mathbb{A} \) to Theorem 5.4. Since the equality (5.2) implies (5.1) for \( \mathcal{F} = \mathcal{S} \), it suffices to show (5.2). To obtain it from Theorem 5.4, we need to show that \((-1)^{m-1} q_m(t)^{m(m+1)/2} \to \exp(\pi it)\) as \( m \to \infty \).
Set \((-1)^{m-1} q_m(t)^{m(m+1)/2} = 1 + \sum_{l \geq 1} \alpha_l(m) t^l\). From Proposition A.1 and Lemma A.3, we see that

\[
\alpha_l(m) = \frac{1}{l} \sum_{j_1+j_2+j_3=l-1 \atop j_1,j_2,j_3 \geq 0} B_{l,j_1,j_2,j_3} \frac{(2\pi i)^{l-j_3}}{j_3!} \left( \frac{j_3}{j_2} \right) (1 + O(m^{-1})) \frac{1}{j_3!} \frac{(m(m+1))^{j_3+1}}{2}
\]

We obtain

\[
= \frac{1}{l} \sum_{j_1+j_2+j_3=l-1 \atop j_1,j_2,j_3 \geq 0} B_{l,j_1,j_2,j_3} \frac{2^{j_1}(\pi i)^{l-j_2}}{j_3!} \frac{(m+1)^{j_3+1}}{m!} \left( \frac{j_3}{j_2} \right) (1 + O(m^{-1}))
\]

\[
= \frac{(\pi i)^l}{l!} (1 + O(m^{-1})).
\]

Thus we find that \(\lim_{m \to \infty} (-1)^{m-1} q_m(t)^{m(m+1)/2} = \exp(\pi i t)\). \(\square\)

### B.3. Proof of cyclic sum formulas.

**Proof of Theorem 5.7.** Our proof is adapted from [Bra05-1, §5], [OO07, §2] and [Kaw19, §5]. We first show (5.3). Set

\[
S_p(k_1, \ldots, k_d; l) = \sum_{p > m_1 > \cdots > m_d+1 \geq 1} \frac{q^{(k_1-1)m_1}}{[m_1]^{k_1-1}} \prod_{j=2}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{k_j}} \frac{q^{(l-1)m_{d+1}}}{[m_{d+1}]^l} \frac{q^{m_1}}{[m_1-m_{d+1}]},
\]

\[
T_p(k_1, \ldots, k_d) = \sum_{p > m_1 > \cdots > m_d > m_{d+1} \geq 0} \prod_{j=1}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{k_j}} \frac{q^{m_{d+1}-m_{d+1}}}{[m_1-m_{d+1}]}.
\]

For \(0 \leq s \leq k_1 - 2\), using

\[(\text{B.2}) \quad \frac{[m_{d+1}]}{[m_1]} \frac{q^{m_{d+1}-m_{d+1}}}{[m_1-m_{d+1}]} = \frac{1}{[m_1-m_{d+1}]} - \frac{1}{[m_1]},\]

we obtain

\[
S_p(k_1, \ldots, k_d; s) = S_p(k_1, \ldots, k_d; s+1) - H_{p-1}(k_1-s, k_2, \ldots, k_d, s+1; q).
\]

Hence

\[
S_p(k_1, \ldots, k_d; 0) = S_p(k_1, \ldots, k_d; k_1-1) - \sum_{s=0}^{k_1-2} H_{p-1}(k_1-s, k_2, \ldots, k_d, s+1; q).
\]

Note that this is true also in the case of \(k_1 = 1\). On the other hand, decomposing \(m_{d+1} \geq 0\) in the summation of \(T_p(k_1, \ldots, k_d)\) into either \(m_{d+1} > 0\) and \(m_{d+1} = 0\), we get

\[
S_p(k_1, \ldots, k_d; 0) = T_p(k_1, \ldots, k_d) - H_{p-1}(k_1+1, k_2, \ldots, k_d).
\]
Using
\[
\frac{[m_{d+1}]}{[m_1]} \frac{q^{m_1-m_{d+1}}}{[m_1-m_{d+1}]} = \frac{q^{m_1-m_{d+1}}}{[m_1]} - \frac{q^{m_1}}{[m_1]},
\]
we see that
\[
\sum_{m_1=m_2+1}^{p-1} \frac{[m_{d+1}]}{[m_1]} \frac{q^{m_1-m_{d+1}}}{[m_1-m_{d+1}]} = \sum_{n=0}^{m_{d+1}-1} \frac{q^{m_2-n}}{[m_2-n]} - \sum_{n=1}^{m_{d+1}} \frac{q^{p-n}}{[p-n]}.
\]
Hence
\[
S_p(k_1, \ldots, k_d; k_1-1) = \sum_{p>m_1>\cdots>m_{d+1}>0} \prod_{j=2}^{d} \frac{q^{(k_j-1)m_j} q^{(k_1-1)m_{d+1}} [m_{d+1}] [m_1]}{[m_j]^k_j} \frac{q^{m_1-m_{d+1}}}{[m_1-m_{d+1}]}
\]
\[
= \sum_{p>m_2>\cdots>m_{d+1}>0} \prod_{j=2}^{d} q^{(k_j-1)m_j} q^{(k_1-1)m_{d+1}} \left( \sum_{n=0}^{m_{d+1}-1} \frac{q^{m_2-n}}{[m_2-n]} - \sum_{n=1}^{m_{d+1}} \frac{q^{p-n}}{[p-n]} \right)
\]
\[
= T_p(k_2, \ldots, k_d, k_1) - V_p(k_2, \ldots, k_d, k_1),
\]
where we put
\[
V_p(k_2, \ldots, k_d, k_1) = \sum_{p>m_2>\cdots>m_{d+1}>m_1\geq 1} \prod_{j=2}^{d} \frac{q^{(k_j-1)m_j} q^{(k_1-1)m_{r+1}} [m_{r+1}] [m_1]}{[m_j]^k_j} \frac{q^{p-m_1}}{[p-m_1]}.
\]
As a consequence we get
\[
T_p(k_1, \ldots, k_d) - T_p(k_2, \ldots, k_d, k_1)
\]
\[
= H_{p-1}(k_1 + 1, k_2, \ldots, k_d; q) - \sum_{s=0}^{k_1-2} H_{p-1}(k_1 - s, k_2, \ldots, k_d, s+1; q)
\]
\[
- V_p(k_2, \ldots, k_d, k_1).
\]
Since \(\sum_{k \in \alpha} (T_p(k) - T_p(k^1, k_1)) = 0\), it holds that
\[
\sum_{k \in \alpha} \left\{ \sum_{s=0}^{k_1-2} H_{p-1}(k_1 - s, k^1, s+1; q) - H_{p-1}(k_1 + 1, k^1; q) \right\} = - \sum_{k \in \alpha} V_p(k^1, k_1).
\]
Using (2.7) and (B.1), we find that
\[
V_p(k^1, k_1) = - \sum_{l=0}^{n-1} ((q^p)^{-1}[p])^l
\]
\[
\times \left\{ H_{p-1}(k^1, k_1, l+1; q) + H_{p-1}(k^1, k_1 + l + 1; q) + (1 - q) H_{p-1}(k^1, k_1 + l; q) \right\}
\]
in $Z_{p,n}$. This completes the proof of (5.3).

For the proof of (5.4), set

$$B_p(k_1, \ldots, k_d; l) = \sum_{p > m_1 \geq \cdots \geq m_{d+1} > 0 \atop m_1 \neq m_{d+1}} \frac{q^{(k_1-1)m_1}}{[m_1]^{k_1-l}} \prod_{j=2}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{m_j}} \frac{q^{(l-1)m_{d+1}}}{[m_{d+1}]^{l}} \frac{q^{m_1}}{[m_1 - m_{d+1}]},$$

$$C_p(k_1, \ldots, k_d) = \sum_{p > m_1 \geq \cdots \geq m_{d+1} > 0 \atop m_1 \neq m_{d+1}} \prod_{j=1}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{m_j}} \frac{q^{m_1 - m_{d+1}}}{[m_1 - m_{d+1}]}.$$

It follows from (B.2) that

$$B_p(k_1, \ldots, k_d; s) = B_p(k_1, \ldots, k_d; s + 1) - H_{p-1}^*(k_1 - s, k_2, \ldots, k_d, s + 1; q) + \sum_{p > m > 0} \frac{q^{(k-d)m}}{[m]^{k+1}}$$

for $0 \leq s \leq k_1 - 2$, where $k = \sum_{j=1}^d k_j$. Hence

$$B_p(k_1, \ldots, k_d; 0) = B_p(k_1, \ldots, k_d; k_1 - 1) - \sum_{l=0}^{k_1-2} H_{p-1}^*(k_1 - l, k_2, \ldots, k_d, l + 1; q)$$

$$+ (k_1 - 1) \sum_{p > m > 0} \frac{q^{(k-d)m}}{[m]^{k+1}}.$$

We have

$$B_p(k_1, \ldots, k_d; 0) = C_p(k_1, \ldots, k_d).$$

On the other hand, by (B.3) we see that

$$\sum_{m_1 = m_2}^{m_1 = m_2+1} \frac{m_{d+1}}{[m_1]} \frac{q^{m_1 - m_{d+1}}}{[m_1 - m_{d+1}]} = \sum_{n=1}^{m_{d+1}} \frac{q^{m_2 - n}}{[m_2 - n]} - \sum_{n=1}^{m_{d+1}} \frac{q^{p-n}}{[p-n]},$$

$$\sum_{m_1 = m_2+1}^{m_1 = m_2+1} \frac{m_2}{[m_1]} \frac{q^{m_1 - m_2}}{[m_1 - m_2]} = \sum_{n=0}^{m_2} \frac{q^{m_2 - n}}{[m_2 - n]} - \sum_{n=1}^{m_2} \frac{q^{p-n}}{[p-n]}.$$

They imply that

$$B_p(k_1, \ldots, k_d; k_1 - 1)$$

$$= \sum_{p > m_1 \geq \cdots \geq m_{d+1} > 0 \atop m_1 \neq m_{d+1}} \prod_{j=2}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{k_j}} \frac{q^{(k_1-1)m_{d+1}}}{[m_{d+1}]^{m_{d+1}}} \frac{q^{m_1 - m_{d+1}}}{[m_1 - m_{d+1}]}.$$
Likewise we see that

\[ W_{m+1} = \sum_{p>m_2 \geq \ldots \geq m_{d+1} > 0} \prod_{j=2}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{k_j}} \frac{q^{(k_1-1)m_{d+1}}}{[m_{d+1}]^{k_1}} \left( \sum_{n=1}^{m_{d+1}} \frac{q^{m_{d-n}}}{[m_2 - n]} - \sum_{n=1}^{m_{d+1}} \frac{q^{p-n}}{[p - n]} \right) \]

\[ + \sum_{p-1 > m_2 = \ldots = m_{d+1} > 0} \prod_{j=2}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{k_j}} \frac{q^{(k_1-1)m_{d+1}}}{[m_{d+1}]^{k_1}} \left( \sum_{n=0}^{m_{d-1}} \frac{q^{m_{d-n}}}{[m_2 - n]} - \sum_{n=1}^{m_{d+1}} \frac{q^{p-n}}{[p - n]} \right) \]

\[ = C_p(k_2, \ldots, k_d, k_1) + \sum_{p>m>0} \frac{q^{(k+1-d)m}}{[m]^{k+1}} - W_p(k_2, \ldots, k_d, k_1), \]

where

\[ W_p(k_2, \ldots, k_d, k_1) = \sum_{p>m_2 \geq \ldots \geq m_{d+1} \geq m_1 > 0} \prod_{j=2}^d \frac{q^{(k_j-1)m_j}}{[m_j]^{k_j}} \frac{q^{(k_1-1)m_{d+1}}}{[m_{d+1}]^{k_1}} \frac{q^{p-m_1}}{[p - m_1]}. \]

Thus we get

\[ C_p(k_1, \ldots, k_d) - C_p(k_2, \ldots, k_d, k_1) \]

\[ = - \sum_{s=0}^{k_1-2} H_{p-1}^s(k_1 - s, k_2, \ldots, k_d, s + 1; q) - W_p(k_2, \ldots, k_d, k_1) \]

\[ + (q - 1) \sum_{p > m > 0} \frac{q^{(k-d)m}}{[m]^k} + k_1 \sum_{p > m > 0} \frac{q^{(k-d)m}}{[m]^{k+1}} \]

Therefore

\[ \sum_{k \in \alpha} \sum_{s=0}^{k_1-2} H_{p-1}^s(k_1 - s, k^1, s + 1; q) \]

\[ = - \sum_{k \in \alpha} W_p(k^1, k_1) + |\alpha|(q - 1) \sum_{p > m > 0} \frac{q^{(k-d)m}}{[m]^k} + \frac{k_1}{d} |\alpha| \sum_{p > m > 0} \frac{q^{(k-d)m}}{[m]^{k+1}}. \]

One computes

\[ \frac{q^{(k-d)m}}{[m]^k} = \frac{q^{(k-d)m}}{[m]^k} ((1 - q^m) + q^m)^{d-1} = \sum_{l=0}^{d-1} \binom{d-1}{l} (1 - q)^l \frac{q^{(k-l-1)m}}{[m]^{k-l}}. \]

Likewise we see that

\[ \frac{q^{(k-d)m}}{[m]^{k+1}} = \sum_{l=0}^{d-1} \binom{d}{l} (1 - q)^l \frac{q^{(k-l)m}}{[m]^{k-l+1}}. \]

Now the desired equality is obtained by applying the expansion (B.1) to \( W_p(k^1, k_1). \)

\[ \square \]
Proof of Corollary 5.8. Since $\phi_{p^k}(q^\pm p) = 1$, applying Theorems 4.3 and 4.4 to Theorem 5.7, we get the desired formulas. □

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(Y. Takeyama) Department of Mathematics, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan

*Email address*: takeyama@math.tsukuba.ac.jp

(K. Tasaka) Department of Information Science and Technology, Aichi Prefectural University, Nagakute, Aichi 480-1198, Japan

*Email address*: tasaka@ist.aichi-pu.ac.jp