RELATIONS OF MULTIPLE ZETA VALUES 
AND THEIR ALGEBRAIC EXPRESSION

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Abstract. We establish a new class of relations among the multiple zeta values
\[
\zeta(k_1, \ldots, k_l) = \sum_{n_1 > \cdots > n_l \geq 1} \frac{1}{n_1^{k_1} \cdots n_l^{k_l}},
\]
which we call the cyclic sum identities. These identities have an elementary proof, 
and imply the “sum theorem” for multiple zeta values. They also have a succinct 
statement in terms of “cyclic derivations” as introduced by Rota, Sagan and Stein. 
In addition, we discuss the expression of other relations of multiple zeta values via 
the shuffle and “harmonic” products on the underlying vector space \( H \) the noncom-
mutative polynomial ring \( \mathbb{Q} \langle x, y \rangle \), and also using an action of the Hopf algebra of 
 quasi-symmetric functions on \( \mathbb{Q} \langle x, y \rangle \).

1. Multiple zeta values. Let \( k_1, k_2, \ldots, k_l \) be positive integers with \( k_1 > 1 \). The 
multiple zeta value \( \zeta(k_1, k_2, \ldots, k_l) \) (of weight \( k_1 + \cdots + k_l \) and length \( l \)) associated 
with this sequence is the sum of the convergent \( l \)-fold infinite series
\[
\sum_{n_1 > n_2 > \cdots > n_l \geq 1} \frac{1}{n_1^{k_1} n_2^{k_2} \cdots n_l^{k_l}}.
\]

These quantities were introduced under the name “multiple harmonic series” in 
[10], and independently (with an opposite convention for the order of the sequence) 
in [21]. They have appeared in knot theory [15], quantum field theory [4], and in 
connection with mirror symmetry [12]. There are many relations among multiple 
zeta values (henceforth MZVs), starting with the widely known and often rediscover-
ered identity \( \zeta(2, 1) = \zeta(3) \). An outstanding example is the “sum theorem”, which 
says that the sum of all MZVs of fixed length and weight is independent of length, 
i.e.
\[
\sum_{\{(k_1, \ldots, k_l) | k_1 + \cdots + k_l = n, k_1 > 1\}} \zeta(k_1, k_2, \ldots, k_l) = \zeta(n).
\]
This was conjectured in [10] and proved independently by A. Granville [8] and D. Zagier. Many other identities have been conjectured and proved in the last decade [2,3,5,15,17,18], but surprising new ones continue to appear. In this paper we establish a new class of relations of MZVs, which can be stated as follows.

**Cyclic sum theorem.** For any positive integers \(k_1, k_2, \ldots, k_l\) with some \(k_i \geq 2\),

\[
(1) \quad \sum_{j=1}^{l} \zeta(k_j + 1, k_j + 1, \ldots, k_j, k_1, \ldots, k_{j-1}) = \sum_{\{j\mid j \geq 2\}} \sum_{q=0}^{k_j-2} \zeta(k_j - q, k_j + 1, \ldots, k_i, k_1, \ldots, k_{j-1}, q + 1).
\]

The name we have given this result will be clearer if we state it in an alternative form using the “duality” of MZVs. If \(s = (k_1, \ldots, k_l)\) is an admissible sequence of positive integers (i.e., \(k_1 > 1\)) with sum \(n\), its dual sequence \(\tau(s) = (j_1, \ldots, j_{n-l})\) (having sum \(n\) and \(j_1 > 1\)) is defined as follows. Let \(\Sigma\) be the map that takes a sequence to its sequence of partial sums, and let \(\Pi_n\) be the set of strictly increasing sequences of positive integers with last element at most \(n\). Set \(\tau(s) = \Sigma^{-1}C_nR_n\Sigma(s)\), where for \((a_1, \ldots, a_i) \in \Pi_n\),

\[
R_n(a_1, \ldots, a_i) = (n - 1 - a_i, n + 1 - a_{i-1}, \ldots, n + 1 - a_1)
\]

and \(C_n(a_1, \ldots, a_i)\) is the complement of \(\{a_1, \ldots, a_i\}\) in \(\{1, 2, \ldots, n\}\) arranged in increasing order. Then \(\tau\) is an involution on the set of admissible positive-integer sequences. Now call two sequences of positive integers cyclically equivalent if one is a cyclic permutation of the other, and let \(\Pi(n, l)\) be the set of cyclic equivalence classes of (not necessarily admissible) positive-integer sequences of sum \(n\) and length \(l\). For the juxtaposition \(s_1s_2\) of two admissible sequences one has \(\tau(s_1s_2) = \tau(s_2)\tau(s_1)\) (see [10], Proposition 3.1), so \(\tau(s')\) is a cyclic permutation of \(\tau(s)\) when \(s'\) is an (admissible) cyclic permutation of \(s\), and thus any equivalence class \(\langle s \rangle \in \Pi(n, l)\) has a dual equivalence class \(\langle \tau(s) \rangle \in \Pi(n, n - l)\). (For example, \(\{(2, 3), (3, 2)\} \in \Pi(5, 2)\) has dual equivalence class \(\{(2, 1, 2), (1, 2, 2), (2, 2, 1)\} \in \Pi(5, 3)\).) The cyclic sum theorem can be restated as follows: for any admissible sequence \(s = (k_1, \ldots, k_l)\) with \(k_1 + \cdots + k_l = n\),

\[
(2) \quad \sum_{(p_1, \ldots, p_l) \in \langle s \rangle} \zeta(p_1 + 1, p_2, \ldots, p_l) = \sum_{(q_1, \ldots, q_{n-l}) \in \langle \tau(s) \rangle} \zeta(q_1 + 1, q_2, \ldots, q_{n-l}).
\]

(For the equivalence of the two forms, see the remarks following Theorem 2.3 below.)

The cyclic sum theorem has an elementary proof involving partial fractions, but admits a remarkably simple expression in terms of “cyclic derivations” (in the sense of [20]) of the noncommutative polynomial algebra \(Q(x, y)\). In this way it parallels an earlier result (Theorem 5.1 of [10], reformulated as Theorem 2.1 below), which was proved by an enlivening partial-fractions argument but can be expressed very simply in terms of ordinary derivations of \(Q(x, y)\). The cyclic sum theorem also implies the sum theorem, giving a new proof of this result which does not involve generating functions as used by Granville and Zagier.

We introduce our algebraic machinery in §2: as in [11], we think of MZVs as images of monomials under a map \(\zeta: \mathfrak{S}^0 \to \mathbb{R}\), where \(\mathfrak{S}^0\) is an appropriate subspace.
of $Q(x, y)$. We define derivations and cyclic derivations of $Q(x, y)$ that give rise to identities of MZVs, and show how the cyclic sum theorem implies the sum theorem. In §3 we prove the cyclic sum theorem by elementary methods. In §4 we return to our algebraic viewpoint, recalling the shuffle and “harmonic” products on $\mathfrak{F}^0$ (both of which make $\zeta$ a homomorphism), and relating them to Theorem 2.1. In §5 we introduce an action of the Hopf algebra $Q\text{Sym}$ of quasi-symmetric functions on $Q(x, y)$. We show how Theorem 2.1, the cyclic sum theorem, and the identities proved by the second author in [17] can be expressed in terms of this action.

The first author conjectured the cyclic sum theorem in August 1999, and thanks Michael Bigotte for checking it by computer against tables of known relations [1] through weight 12. The second author proved the conjecture during his stay at the Max-Planck-Institut für Mathematik in Bonn in early 2000, and he thanks Masanobu Kaneko and Don Zagier for useful discussions and the Institut for its hospitality. The second author is supported in part by the Research Fellowship of the Japan Society for the Promotion of Science for Young Scientists.

2. A noncommutative polynomial algebra and its derivations. In this section we introduce an algebraic approach by thinking of MZVs as values of a homomorphism from a subspace of the noncommutative polynomial algebra $Q(x, y)$ to the reals. We then consider both derivations and “cyclic derivations” (defined below) of $Q(x, y)$, and formulate relations of MZVs in terms of them. We state the cyclic sum theorem algebraically (Theorem 2.3), show it is equivalent to the two forms (1) and (2) given in §1, and finally prove the sum theorem from the cyclic sum theorem.

Let $Q(x, y)$ be the algebra of polynomials over the rationals in noncommutative indeterminates $x, y$, regarded as a graded $Q$-algebra with $x$ and $y$ both of degree 1. For any word (monomial) $w$ of $Q(x, y)$, denote by $|w|$ its total degree (also called its weight) and by $\ell(w)$ the number of occurrences of $y$ in $w$ (called the length of $w$). We call $|w| - \ell(w)$ the coelastic of $w$: it is the number of occurrences of $x$ in $w$. The underlying graded rational vector space of $Q(x, y)$ is denoted $\mathfrak{H}$.

Let $\mathfrak{H}^1 = Q1 \oplus \mathfrak{H}y$ and $\mathfrak{H}^0 = Q1 \oplus x\mathfrak{H}y$. Then $\mathfrak{H}^1$ is a subalgebra of $Q(x, y)$, in fact the noncommutative polynomial algebra on generators $z_i = x^{l_i}y$. We have $\mathfrak{H} = \mathfrak{H}x \oplus \mathfrak{H}^1$ and $\mathfrak{H}^2 = y\mathfrak{H}^1 \oplus \mathfrak{H}^0$. We can think of MZVs as images of words of $Q(x, y)$ under the $Q$-linear map $\zeta : \mathfrak{H}^0 \to \mathbb{R}$ defined by $\zeta(1) = 1$ and

$$\zeta(x^{k_1-1}y^{k_2-1} \cdots x^{k_l-1}y) = \zeta(k_1, k_2, \ldots, k_l)$$

for any positive integers $k_1, k_2, \ldots, k_l$ with $k_1 > 1$.

Let $\tau$ be the anti-automorphism of $Q(x, y)$ exchanging $x$ and $y$, e.g. $\tau(x^2yxy) = xyxy^2$. Evidently $\tau$ is an involution. Applied to words, $\tau$ preserves weight and exchanges length and colength: note that $\mathfrak{H}^0$ (but not $\mathfrak{H}^1$) is closed under $\tau$. It is easy to check that for dual sequences $s = (k_1, \ldots, k_l)$ and $s = (j_1, \ldots, j_{n-l})$ as defined in the preceding section, $\tau(x^{k_1-1}y^{k_2-1} \cdots x^{k_l-1}y) = x^{n-l-1}y^{j_1} \cdots x^{j_{n-l-1}-1}y$.

As usual, by a derivation of $Q(x, y)$ we mean a map $F : \mathfrak{H} \to \mathfrak{H}$ (of graded rational vector spaces) such that $F(uv) = F(u)v + uF(v)$ for all $u, v \in \mathfrak{H}$. The commutator of two derivations is a derivation, so the set of derivations of $Q(x, y)$ is a Lie algebra graded by degree. If $\delta$ is a derivation, then $\bar{\delta} = \tau \delta \tau$ is also a derivation (of the same degree). We call a derivation $\delta$ symmetric if $\bar{\delta} = \delta$ and antisymmetric if $\bar{\delta} = -\delta$.

Since $[\delta, \varepsilon] = [\bar{\delta}, \varepsilon]$ symmetric and antisymmetric derivations behave nicely under commutator, e.g. $[\delta, \varepsilon]$ is antisymmetric if $\delta$ is symmetric and $\varepsilon$ antisymmetric.
Note that a symmetric or antisymmetric derivation is completely determined by where it sends $x$.

We denote by $D$ the derivation such that $D(x) = 0$ and $D(y) = xy$. In terms of the generators $z_i$ of $\mathfrak{H}^1$ mentioned above, we have $D(z_i) = z_{i+1}$ and more generally

$$\tag{3} D(z_{i_1}z_{i_2} \cdots z_{i_l}) = z_{i_1+1}z_{i_2} \cdots z_{i_l} + z_{i_1}z_{i_2+1}z_{i_3} \cdots z_{i_l} + \cdots + z_{i_1} \cdots z_{i_{l-1}}z_{i_l+1}.$$ 

The following result was proved by a partial-fractions argument in [10]. We note that the hypothesis on $w$ cannot be weakened, since $\zeta(D(y)) = \zeta(xy) \neq 0 = \zeta(\bar{D}(y))$.

Theorem 2.1. For any word $w$ of $\mathfrak{H}^0$, $\zeta(D(w)) = \zeta(\bar{D}(w))$.

K. Ihara and M. Kaneko [13] have generalized Theorem 2.1 as follows. For $n \geq 1$ let $\partial_n$ be the antisymmetric derivation with $\partial_n(x) = x(x+y)^{n-1}y$; note that $\partial_1 = \bar{D} - D$.

Theorem (Ihara and Kaneko). For all $n \geq 1$ and words $w$ of $\mathfrak{H}^0$, $\zeta(\partial_n(w)) = 0$.

We shall discuss the proof of this result in §5 below.

We now consider cyclic derivations of $\mathbb{Q}(x,y)$; these are not derivations, but rather are defined as follows (cf. [20]).

Definition. A cyclic derivation $\psi$ of $\mathbb{Q}(x,y)$ is a $\mathbb{Q}$-linear map $\psi : \mathfrak{H} \to \text{End} \mathfrak{H}$, where $\text{End} \mathfrak{H}$ is the graded rational vector space of endomorphisms of $\mathfrak{H}$ (as a graded rational vector space), such that

$$\tag{4} (\psi(f_1f_2), f) = (\psi(f_1), f_2f) + (\psi(f_2), f_1f)$$

for all $f_1, f_2, f \in \mathfrak{H}$, where $(\beta, u)$ denotes the image of $u \in \mathfrak{H}$ under $\beta \in \text{End} \mathfrak{H}$.

If $\psi$ is a cyclic derivation, evidently $\psi(1)$ is the zero endomorphism. By induction equation (4) is easily extended to the identity

$$\tag{5} (\psi(f_1f_2 \cdots f_n), f) = (\psi(f_1), f_2 \cdots f_nf) + (\psi(f_2), f_3 \cdots f_nf f_1) + \cdots + (\psi(f_n), f_1f \cdots f_{n-1})$$

(cf. Proposition 2.3 of [20]; unfortunately the statement has a misprint).

Just as the conjugate by $\tau$ of an ordinary derivation is a derivation, it is possible to conjugate a cyclic derivation by $\tau$ as follows.

Proposition 2.2. Suppose $\psi$ is a cyclic derivation. Then the map $\bar{\psi} : \mathfrak{H} \to \text{End} \mathfrak{H}$

is also a cyclic derivation, where

$$\bar{\psi}(f)(g) = \tau(\psi(\tau(f)), \tau(g))$$

for $f, g \in \mathfrak{H}$.

Proof. It suffices to check identity (4), which is routine. □

If $\psi$ is a cyclic derivation and $f \in \mathfrak{H}$, the endomorphism $\psi(f)$ gives rise to a canonical element $(\psi(f), 1)$ of $\mathfrak{H}$; we shall abuse notation and write $\psi(f)$ for this element of $\mathfrak{H}$ when no confusion can arise. Note that as elements of $\mathfrak{H}$, $\psi(fg) = \psi(gf)$ and $\bar{\psi}(f) = \tau(\psi(f))$ for any $f, g \in \mathfrak{H}$.
Now we define the cyclic derivation \( C \) of \( \mathbf{Q}(x, y) \) by setting \( C(x) = 0 \) (zero endomorphism) and \( (C(y), f) = xf y \) for all \( f \in \mathcal{H} \). By applying identity (5), it is easy to see that

\[
(C(z_i), f) = (C(x^{i-1} y), f) = (C(y), f x^{i-1}) = x f x^{i-1} y = x f z_i
\]

for \( f \in \mathcal{H} \), and thus (abusing notation as indicated above) that \( C(z_i) = z_{i+1} \). Given an arbitrary monomial \( w = z_i z_{i+1} \cdots z_l \) of \( \mathcal{H}^1 \), we can apply identity (5) to get

\[
C(w) = z_{i+1} z_{i+2} \cdots z_l + z_{i+1} z_{i+2} \cdots z_l z_{i+1} + \cdots + z_{i+1} z_{i+2} \cdots z_{l-1},
\]

which may be compared to equation (3). Similarly, it can be shown that

\[
\bar{C}(z_i z_{i+1} \cdots z_l) = \sum_{i_j \geq 2} \sum_{q=0}^{i_j-2} z_{i_j-q} z_{i_{j+1}} \cdots z_{i_j} z_{i_{j+1}} \cdots z_{i_{j+1}},
\]

Thus, form (1) of cyclic sum theorem as stated in \( \S 1 \) may be expressed as follows; the proof is given in \( \S 3 \) below.

**Theorem 2.3.** For any word \( w \) of \( \mathcal{H}^1 \) that is not a power of \( y \), \( \zeta(C(w)) = \zeta(\bar{C}(w)) \).

Let \( s = (k_1, \ldots, k_l) \) be an admissible sequence of positive integers, and \( w = x^{k_1-1} y \cdots x^{k_l-1} y \) the corresponding word of \( \mathcal{H}^0 \). In view of equation (6),

\[
\zeta(C(w)) = m(w) \sum_{(p_1, \ldots, p_l) \in [s]} \zeta(p_1 + 1, p_2, \ldots, p_l),
\]

where \([s]\) is the equivalence class of \( s \) in \( \Pi(k_1 + \cdots + k_l, l) \) and \( m(w) \) is the largest integer \( m \) such that \( w = u^m \) for \( u \in \mathcal{H}^1 \). Then form (2) of the cyclic sum theorem is equivalent to \( \zeta(C(w)) = \zeta(C(\tau(w))) \) (note \( m(\tau(w)) = m(w) \)), and this is equivalent to Theorem 2.3 since \( \zeta \) is \( \tau \)-invariant (see Theorem 4.1 below).

Theorems 2.1 and 2.3 are of course formally very similar. Both give an equation between a sum of MZVs of length \( l \) and a sum of MZVs of length \( l+1 \). An important difference between the two results is that \( C \) is much simpler than \( D \) on periodic words of \( \mathcal{H}^0 \). For example, Theorem 2.3 applied to \( z_n^l \) gives

\[
\zeta(z_{n+1} z_n^{l-1}) = \sum_{i=0}^{n-2} \zeta(z_{n-i} z_n^{l-1} z_{i+1}).
\]

In the sequence notation, the case \( n = 3 \) is

\[
\zeta(4, 3, \ldots, 3) = \zeta(3, 3, \ldots, 3, 1) + \zeta(2, 3, \ldots, 3, 2),
\]

which does not seem to follow easily from other known identities. We close this section by deducing the sum theorem from the cyclic sum theorem.
Corollary 2.4. For any integers $1 \leq l < n$, let $S(n, l)$ be the sum of words $w \in \mathcal{F}_0$ with $|w| = n$ and $\ell(w) = l$. Then $\sum_{w \in S(n, l)} \zeta(w)$ is independent of $l$ (and, in particular, is equal to $\zeta(z_n) = \zeta(n)$).

Proof. Consider the element $\mu = (x + ty)^{n-1} - x^{n-1} - t^{n-1}y^{n-1} \in \mathcal{F}_0[t]$. From the properties of cyclic derivation (cf. Corollary 2.5 of [20]) we have

$$C((x + ty)^{n-1}) = (C((x + ty)^{n-1}), 1) = (n - 1)C(x + ty, (x + ty)^{n-2}) = (n - 1)tx(x + ty)^{n-2}y,$$

and thus $C(\mu) = (n - 1)(tx(x + ty)^{n-2}y - t^{n-1}xy^{n-1})$; a similar calculation gives $C(\mu) = (n - 1)(x(x + ty)^{n-2}y - x^{n-1}y)$. For each $1 \leq l < n - 1$, the coefficient of $t^l$ in $\zeta(C(\mu) - C(\mu))$ gives the identity

$$\sum_{w \in S(n, l)} \zeta(w) - \sum_{w \in S(n, l+1)} \zeta(w) = 0$$

after dividing by $n - 1$. $\square$

3. Proof of the cyclic sum theorem. For positive integers $k_1, k_2, \ldots, k_l$ and nonnegative integer $k_{l+1}$, let

$$T(k_1, \ldots, k_l) = \sum_{n_1 > n_2 > \cdots > n_i > n_{i+1} \geq 0} \frac{1}{(n_1 - n_{l+1})n_1^{k_1} \cdots n_l^{k_l}}$$

and

$$S(k_1, \ldots, k_l, k_{l+1}) = \sum_{n_1 > n_2 > \cdots > n_i > n_{i+1} > 0} \frac{1}{(n_1 - n_{l+1})n_1^{k_1} \cdots n_l^{k_l} n_{l+1}^{k_{l+1}}}.$$

For the convergence of these series, we have the following.

Theorem 3.1. $T(k_1, \ldots, k_l)$ is bounded when one of $k_1, \ldots, k_l$ exceeds 1, and $S(k_1, \ldots, k_l, k_{l+1})$ is bounded when one of $k_1, \ldots, k_l, k_{l+1} + 1$ exceeds 1.

Our key result is as follows.

Theorem 3.2. For any positive integers $k_1, k_2, \ldots, k_l$ with $k_i > 1$ for some $i$,

$$T(k_1, \ldots, k_i) - T(k_2, \ldots, k_i, k_1) = \zeta(k_1 + 1, k_2, \ldots, k_l) - \sum_{j=0}^{k_1-2} \zeta(k_1 - j, k_2, \ldots, k_l, j+1)$$

where the sum on the right is understood as 0 if $k_1 = 1$.

To prove the cyclic sum theorem in the form stated in §1, sum Theorem 3.2 over all cyclic permutations of the sequence $(k_1, \ldots, k_l)$.

It is immediate that

(7) $S(k_1, \ldots, k_l, 0) = T(k_1, \ldots, k_l) - \zeta(k_1 + 1, k_2, \ldots, k_l)$.

Also, applying the identity

(8) $\frac{1}{n_1(n_1 - n_{l+1})} = \frac{1}{n_{l+1}} \left( \frac{1}{n_1 - n_{l+1}} - \frac{1}{n_1} \right)$
to \( S(k_1, \ldots, k_l, k_{l+1}) \) gives

\[ S(k_1, \ldots, k_l, k_{l+1}) = S(k_1 - 1, k_2, \ldots, k_l, k_{l+1} + 1) - \zeta(k_1, \ldots, k_l, k_{l+1} + 1). \]

Finally, applying (8) to \( S(1, k_2, \ldots, k_l, k_{l+1}) \) gives

\[
\sum_{n_1 > n_2 > \cdots > n_{l+1} > 0} \frac{1}{n_2^{k_2} \cdots n_l^{k_l} n_{l+1}^{k_{l+1}+1}} \left( \frac{1}{n_1 - n_{l+1}} - \frac{1}{n_1} \right) = \\
\sum_{n_1 > n_2 > \cdots > n_{l+1} > 0} \frac{1}{n_2^{k_2} \cdots n_l^{k_l} n_{l+1}^{k_{l+1}+1}} \sum_{n_1 = n_{l+1}+1}^{\infty} \left( \frac{1}{n_1 - n_{l+1}} - \frac{1}{n_1} \right) = \\
\sum_{j=0}^{n_{l+1}-1} \frac{1}{n_2 - j} \cdot \sum_{n_1 > n_2 > \cdots > n_{l+1} > j \geq 0} \frac{1}{(n_2 - j)^{k_2} \cdots n_l^{k_l} n_{l+1}^{k_{l+1}+1}}
\]

and so

\[ S(1, k_2, \ldots, k_l, k_{l+1}) = T(k_2, \ldots, k_l, k_{l+1} + 1). \]

\textit{Proof of Theorem 3.2.} Apply equation (7), then equation (9) \( k_1 - 1 \) times, and finally equation (10):

\[
T(k_1, \ldots, k_l) - \zeta(k_1 + 1, k_2, \ldots, k_l) = S(k_1, \ldots, k_l, 0) = \\
S(k_1 - 1, k_2, \ldots, k_l, 1) - \zeta(k_1, \ldots, k_l, 1) = \cdots = \\
S(1, k_2, \ldots, k_l, k_l - 1) - \sum_{j=0}^{k_l-2} \zeta(k_1 - j, k_2, \ldots, k_l, j + 1) = \\
T(k_2, \ldots, k_l, k_l) - \sum_{j=0}^{k_l-2} \zeta(k_1 - j, k_2, \ldots, k_l, j + 1). \quad \square
\]

\textit{Proof of Theorem 3.1.} Using equation (7),

\[
S(k_1, \ldots, k_l, k_{l+1}) \leq S(k_1, \ldots, k_l, 0) \leq T(k_1, \ldots, k_l),
\]

so \( S(k_1, \ldots, k_{l+1}) \) is bounded if \( T(k_1, \ldots, k_l) \) is; and if \( k_1 = 1 \), equation (10) says \( S(k_1, \ldots, k_{l+1}) = T(k_2, \ldots, k_l, k_{l+1} + 1) \). So the statement about the \( S \)'s follows from the one about the \( T \)'s. Also, to prove the first assertion it is evidently enough to treat the case \( k_1 + \cdots + k_l = l + 1 \). Now

\[
T(2, 1, \ldots, 1) = \\
\sum_{n_1 > n_2 > \cdots > n_{l+1} > 0} \frac{1}{n_1^{n_1}(n_1 - n_{l+1}) n_2 \cdots n_l} \leq \\
\sum_{n_1 > n_2 > \cdots > n_0 > 0} \frac{1}{n_1^{l} j n_2 \cdots n_l} \\
= \zeta(3, 1, \ldots, 1) + l \zeta(2, 1, \ldots, 1) + \sum_{i=1}^{l-1} \zeta(2, 1, \ldots, 1, 2, 1, \ldots, 1) + l\zeta(2, 1, \ldots, 1, 1, \ldots, 1).
so \(T(2,1,\ldots,1)\) is bounded. Then by equations (7) and (10), we have
\[
T(1,2,1,\ldots,1) = S(1,2,1,\ldots,1,0) + \zeta(2,2,1,\ldots,1)
\]
\[
= T(2,1,\ldots,1,1) + \zeta(2,2,1,\ldots,1)
\]
and we can continue in this way to bound all the sums \(T(1,\ldots,1,2,1,\ldots,1)\). □

4. Commutative multiplications on \(\mathfrak{H}\). There are two commutative multiplications on the vector space \(\mathfrak{H}\), both of which have significance for MZVs. First, there is the shuffle product \(\mathfrak{m}\), which can be defined inductively on words of \(\mathfrak{H}\) by requiring that it distribute over addition and satisfy the axioms

S1. for any word \(w\), \(1w = w = w1\);
S2. for any words \(w_1, w_2\) and \(a, b \in \{x, y\},
\[
aw_1bw_2 = a(w_1mbw_2) + b(aw_1mw_2).
\]

It is evident that \((\mathfrak{H}, \mathfrak{m})\) is a subalgebra of \((\mathfrak{H}, \mathfrak{m})\), and we have the following result.

**Theorem 4.1.** \(\zeta\) is a \(\tau\)-invariant homomorphism of \((\mathfrak{H}, \mathfrak{m})\) into \(\mathbb{R}\).

**Proof.** This follows from the representation of MZVs as iterated integrals (see [21,14,11,9]). If we define iterated integrals recursively by
\[
\int_0^t \alpha_1 = \int_0^t f(s)ds
\]
and
\[
\int_0^t \alpha_1\alpha_2\cdots\alpha_n = \int_0^t f(s) \left( \int_0^s \alpha_2\cdots\alpha_n \right) ds
\]
for \(\alpha_1 = f(t)dt\), then it is easy to show that for any nonnegative integers \(p_1, p_2, \ldots, p_t\) with \(p_1 > 1,
\[
\zeta(x^{p_1}y \cdots x^{p_t}y) = \int_0^1 \omega_0^{p_1} \omega_1 \cdots \omega_0^{p_t} \omega_1
\]
where \(\omega_0 = dt/t\) and \(\omega_1 = dt/(1 - t)\). That \(\zeta\) is a homomorphism then follows from the fact that iterated integrals multiply according to shuffle products [19]. The \(\tau\)-invariance follows from a change of variable. □

Second, there is the “harmonic” product \(*\) defined on \(\mathfrak{H}\) by requiring that it distribute over addition and satisfy the axioms

H1. for any word \(w\), \(1 * w = w * 1 = w\);
H2. for any word \(w\) and positive integer \(p\), \(x^p * w = wx^p\);
H3. for any words \(w_1, w_2\) and positive integers \(p, q\),
\[
x^{p-1}yw_1x^{q-1}yw_2 = x^{p-1}y(w_1x^{q-1}yw_2) + x^{q-1}y(x^{p-1}yw_1 + w_2) + x^{p+q-1}y(w_1w_2).
\]

As was shown in [11], this defines a commutative and associative product on \(\mathfrak{H}\). If \(\mathfrak{H}\) is regarded as the underlying vector space of the noncommutative algebra \(\mathbb{Q}(z_1, z_2, \ldots)\), where \(z_i = x^{i-1}y\) as in §2, then axiom (H3) for words of \(\mathfrak{H}\) reads
\[
z_pw_1 * z_qw_2 = z_p(w_1 * z_qw_2) + z_q(z_pw_1 * w_2) + z_{p+q}(w_1 * w_2),
\]
which may be compared to (S2). This can be thought of as describing multiplication of series, and the following result is proved in [11].
Theorem 4.2. The map $\zeta : (\mathcal{H}^0, *) \rightarrow \mathbb{R}$ is a homomorphism.

On the other hand, we can define a $\mathbb{Q}$-linear map from $\phi : \mathcal{H}^1 \rightarrow \mathbb{Q}[t_1, t_2, \ldots]$, where $\mathbb{Q}[t_1, t_2, \ldots]$ is the $\mathbb{Q}$-algebra of formal series in the countable set of (commuting) variables $t_1, t_2, \ldots$, by setting $\phi(1) = 1$ and

$$\phi(z_{i_1} \cdots z_{i_n}) = \sum_{n_1 > n_2 > \cdots > n_1 \geq 1} t_{i_1}^{n_1} t_{i_2}^{n_2} \cdots t_{i_n}^{n_1}.$$ 

Then $\phi$ is a homomorphism, and in fact a monomorphism; its image is the algebra $\text{QSym}$ of quasi-symmetric functions as defined in [7]. A formal power series (of bounded degree) in $t_1, t_2, \ldots$ is a quasi-symmetric function if the coefficients $t_{i_1}^{1} t_{i_2}^{2} \cdots t_{i_k}^{j_k}$ and $t_{i_1}^{j_1} t_{i_2}^{j_2} \cdots t_{i_k}^{j_k}$ are the same whenever $1 < j_2 < \cdots < j_k$. Evidently any quasi-symmetric function is a sum of monomial quasi-symmetric functions, which can be defined as the elements $\phi(z_{i_1} \cdots z_{i_k})$.

Since $\zeta : \mathcal{H}^0 \rightarrow \mathbb{R}$ is a homomorphism for both multiplications, any element of the form $\langle u, v \rangle = umw - u * v$ for $u, v \in \mathcal{H}^0$ must be in the kernel of $\zeta$. Together with Theorem 2.1, our next result shows that this remains true for elements of the form $\langle y, w \rangle$, $w \in 0$. 

Theorem 4.3. For words $w$ of $\mathcal{H}$, $\text{ymw} - y * w = D(w) - D(w)$, where $D$ is the derivation of $\mathcal{H}$.

Proof. We proceed by induction on $\ell(w)$. If $\ell(w) = 0$, then $w = x^k$ and we have

$$\text{ymw} - y * w = yx^k + x^k - yx^k = x^k - x^k = D(x^k) - D(x^k).$$

Now suppose $\ell(w) = n > 0$ and the result holds for words of length less than $n$. Then we can write $w = x_1 y w_1$ for some word $w_1$ with $\ell(w_1) = n - 1$. Using the inductive definitions (S2) and (H3), we have

$$\text{ym}(x^k y w_1) = yx^k y w_1 + x^k y - x^k y y w_1 + x^k w_1,$$

whence, assuming the induction hypothesis, is

$$\langle y, w \rangle = yx^k y w_1 + x^k y w_1 + x^k y (y * w_1),$$

whose difference, using the inductive hypothesis, is

$$x^k y x^{k-1} y w_1 + \cdots + x^k y^2 w_1 - x^k y w_1 + x^k y (D - D)(w_1).$$

On the other hand, since $D - D$ is a derivation, we have

$$(D - D)(x^k y w_1) = x^k y x^{k-1} y w_1 + \cdots + x^k y^2 w_1 - x^k y w_1 + x^k y (D - D)(w_1),$$

which agrees with (11). □

5. Action of the Hopf algebra $\text{QSym}$ on $\mathcal{H}$. In this section we put a Hopf algebra structure on $\mathcal{H}^1 \cong \text{QSym}$, and define an action of this Hopf algebra on $\mathbb{Q}(x, y)$ that is related to the results of the preceding sections. In particular, we state a previous result of the second author in terms of this action, and give a proof of the result of Iwara and Kaneko stated in §2. All the algebraic definitions needed can be found in [14].
Clearly the algebra $\text{QSym}$ of quasi-symmetric functions contains the algebra $\text{Sym}$ of symmetric functions. In fact, the isomorphism $\phi : \mathcal{F}^1 \rightarrow \text{QSym}$ of the preceding section takes $z_n$ to the power-sum symmetric function $p_n = \sum t_i^n$, and $z_i^n$ to the elementary symmetric function $e_n = \sum_{i_1 < \cdots < i_n} t_{i_1} \cdots t_{i_n}$. Further, $\text{QSym}$ can be given a Hopf algebra structure that extends the usual Hopf algebra structure on $\text{Sym}$ (see [6,5]); the primitives are the power-sum symmetric functions $p_n$. If $\Delta : \mathcal{F}^1 \rightarrow \mathcal{F}^1 \otimes \mathcal{F}^1$ is the adjoint of the concatenation product on the generators $z_i$, i.e.

$$\Delta(z_{i_1} z_{i_2} \cdots z_{i_k}) = \sum_{j=0}^k z_{i_1} \cdots z_{i_j} \otimes z_{i_{j+1}} \cdots z_{i_k},$$

then $(\mathcal{F}^1, *, \Delta)$ is a Hopf algebra and the map $\phi : \mathcal{F}^1 \rightarrow \text{QSym}$ is an isomorphism of Hopf algebras. Henceforth we shall identify $(\mathcal{F}^1, *, \Delta)$ with $\text{QSym}$ via $\phi$; so $z_n$ is the $n$th power-sum symmetric function and so forth.

Now define a $\mathbb{Q}$-linear map $\cdot : \mathcal{F}^1 \otimes \mathcal{F} \rightarrow \mathcal{F}$ as follows. Let $1 \cdot w = w$ for any word $w$ of $\mathcal{F}$. For a nonempty word $u$ of $\mathcal{F}^1$, let $u \cdot x = 0$,

$$u \cdot y = \begin{cases} x^k y, & u = z_k, \\ 0, & \text{otherwise}, \end{cases}$$

and

$$(12) \quad u \cdot w_1 w_2 = \sum_u (u' \cdot w_1)(u'' \cdot w_2)$$

for words $w_1, w_2$ of $\mathcal{F}$, where $\Delta(u) = \sum u' \otimes u''$. Then the coassociativity of $\Delta$ implies that $u \cdot w \in \mathcal{F}$ is well-defined for any words $u$ of $\mathcal{F}^1$ and $w$ of $\mathcal{F}$. The following fact is immediate from the definitions.

**Proposition 5.1.** For words $w$ of $\mathcal{F}$, $z_1 \cdot w = D(w)$; more generally, the linear map $D_n : \mathcal{F} \rightarrow \mathcal{F}$ defined by $D_n(w) = z_n \cdot w$ is the derivation sending $x$ to 0 and $y$ to $x^n y$.

The map $\cdot$ is related to the multiplication $*$ of the previous section as follows.

**Lemma 5.2.** For words $u \in \mathcal{F}^1$ and $w \in \mathcal{F}$, $u \cdot w$ is the sum of terms in $u * w$ of length $\ell(w)$.

**Proof.** We proceed by induction on $\ell(w)$. If $\ell(w) \leq 1$ then $w$ is either a power of $x$ or of the form $x^p y x^q$, and the conclusion is clear from the definition. Now suppose the conclusion is true if $\ell(w) < n$ and let $w$ be a word of length $n$. Writing $u = z_i u_1$ and $w = x^{p-1} y w_1$, we have (from axiom (H3) above)

$$u \ast w = z_i (u_1 \ast w) + x^{p-1} y (u \ast w_1) + x^{i+p-1} y (u_1 \ast w_1).$$

Note that only the last two terms can contribute words of length $\ell(w)$. Since $\ell(w_1) < n$, we have by the induction hypothesis

$$\text{sum of terms of length } \ell(w) \text{ in } u \ast w = x^{p-1} y (u \ast w_1) + x^{i+p-1} y (u_1 \ast w_1).$$

But applying equation (12) to $u \cdot w = z_i u_1 \cdot x^{p-1} y w_1$ gives

$$u \cdot w = (1 \cdot x^{p-1} y)(u \cdot w_1) + (z_i \cdot x^{p-1} y)(u_1 \cdot w_1)$$

$$= x^{p-1} y (u \cdot w_1) + x^{i+p-1} y (u_1 \cdot w_1). \quad \Box$$
Theorem 5.3. The map \( \cdot \) : \( \mathcal{H}^1 \otimes \mathcal{H} \to \mathcal{H} \) is an action of the algebra \( \text{QSym} \cong \mathcal{H}^1 \) on \( \mathcal{H} \), and in fact makes \( \mathbb{Q}[x,y] \) a QSym-module algebra.

Proof. It suffices to show that \( u \cdot (v \cdot w) = (u \ast v) \cdot w \) for words \( u, v \) of \( \mathcal{H}^1 \) and \( w \) of \( \mathcal{H} \). But by the lemma, both sides are just the sum of words of length \( \ell(w) \) in \( u \ast (v \ast w) = (u \ast v) \ast w \). \( \square \)

There is a relation between the action and the cyclic derivation \( C \) of \( \S 2 \).

Proposition 5.4. For positive integers \( n, m \), \( C(x^n y^m) = z_n \cdot xy^m \).

Proof. Using identity (5), we have \( (C(y^m), f) = xy^{m-1}fy + xy^{m-2}fy^2 + \cdots + xfy^m \), for any \( f \in \mathcal{H} \), so \( C(x^n y^m) = (C(y^m), x^n) = xy^{m-1}x^n y + xy^{m-2}x^n y^2 + \cdots + x^{n+1}y^m \), and the conclusion follows. \( \square \)

This has the following corollary.

Corollary 5.5. For all \( n, m \geq 1 \), \( \zeta(z_n \cdot xy^m) = \zeta(z_m \cdot xy^n) \).

Proof. By the preceding result, \( z_n \cdot xy^m = C(x^n y^m) \); on the other hand, \( \tau C(x^n y^m) = C(\tau(x^n y^m)) = C(x^m y^n) = z_m \cdot xy^n \), and the conclusion follows from Theorems 2.3 and 4.1. \( \square \)

A result of the second author [17] can be formulated in terms of the QSym-action on \( \mathbb{Q}(x, y) \) as follows. Let \( h_n \) denote the complete symmetric function of degree \( n \), i.e. the sum of all monomials in the \( z_i \) of weight \( n \).

Theorem 5.6. For all integers \( n \geq 0 \) and words \( w \) of \( \mathcal{H}^0 \), \( \zeta(h_n \cdot \tau(w)) = \zeta(h_n \cdot w) \).

In view of Proposition 5.1 (and the \( \tau \)-invariance of \( \zeta \)), Theorem 2.1 is the case \( n = 1 \) of this theorem. In fact, Ihara and Kaneko proved the theorem stated in \( \S 2 \) by showing it equivalent to Theorem 5.6. The argument that follows is based on their proof, but has been recast in terms of the QSym-action.

If we let \( \mathcal{H}[[t]] \) be the ring of formal power series in \( t \) with coefficients in \( \mathcal{H} \), then the action of QSym on \( \mathcal{H} \) extends to an action of QSym[[t]] on \( \mathcal{H}[[t]] \). Since \( p_n = z_n \) acts on \( \mathcal{H} \) as the derivation \( D_n \) of Proposition 5.1, the operator

\[
\sigma_t = \exp \left( \sum_{n=1}^{\infty} \frac{D_n t^n}{n} \right)
\]

is an automorphism of \( \mathcal{H}[[t]] \) by the following result.

Lemma 5.7. Suppose \( \delta = t \delta_1 + t^2 \delta_2 + \cdots \), where each \( \delta_i \) is derivation of \( \mathcal{H} \). Then

\[
\exp(\delta) = \text{id} + t \delta_1 + t^2 \left( \frac{\delta_1^2}{2} + \delta_2 \right) + \cdots
\]
is an automorphism of $\mathcal{Y}[[t]]$.

Proof. First, note that $\delta$ is a derivation of $\mathcal{Y}[[t]]$: given $u = u_0 + tu_1 + t^2u_2 + \cdots$ and $v = v_0 + tv_1 + t^2v_2 + \cdots$ in $\mathcal{Y}[[t]]$, the coefficient of $t^n$ in $\delta(uv)$ is

$$
\sum_{p+q+r=n} \delta_p(u_qv_r) = \sum_{p+q+r=n} (\delta_p(u_q)v_r + u_q\delta_r(v_r));
$$

but this is also the coefficient of $t^n$ in $\delta(u)v + u\delta(v)$. It then follows that $\exp(\delta)$ is an automorphism of $\mathcal{Y}[[t]]$, since for $u, v \in \mathcal{Y}[[t]]$ we have

$$
\exp(\delta)(uv) = \sum_{n \geq 0} \frac{\delta^n(uv)}{n!} = \sum_{n \geq 0} \left( \sum_{i=0}^{\lfloor n/2 \rfloor} \binom{n}{i} \delta^i(u)\delta^{n-i}(v) \right) = \sum_{n \geq 0} \left( \sum_{i+j=n} \frac{\delta^i(u)\delta^j(v)}{i!j!} \right) = \exp(\delta(u))\exp(\delta(v)). \quad \square
$$

Now $H(t) = 1 + h_1t + h_2t^2 + \cdots \in \text{QSym}[[t]]$, and from the well-known identity

$$
\frac{d}{dt} \log H(t) = \frac{H'(t)}{H(t)} = \sum_{n=1}^{\infty} p_n t^{n-1}
$$

(see, e.g., [16]) it follows that $\sigma_t(u) = H(t)\cdot u$ for $u \in \mathcal{Y}[[t]]$. Setting $\bar{\sigma}_t = \tau\sigma_t\tau$, we can restate Theorem 5.6 as saying that $\zeta(\bar{\sigma}_t(w) - \sigma_t(w)) = 0$ for any word $w$ of $\mathcal{Y}^0$, or equivalently (since $\sigma_t(\mathcal{Y}^0) \subset \mathcal{Y}^0[[t]]$)

$$
(13) \quad \bar{\sigma}_t\sigma_t^{-1}(u) - u \in \ker \zeta \quad \text{for all } u \in \mathcal{Y}^0[[t]].
$$

Also, since $H(t)^{-1} = E(-t)$, where $E(t) = 1 + e_1t + e_2t^2 + \cdots = 1 + yt + y^2t^2 + \cdots$, we have $\sigma_t^{-1}(u) = E(-t)\cdot u$.

Lemma 5.8. $\Phi = \bar{\sigma}_t\sigma_t^{-1}$ is uniquely characterized (among automorphisms of $\mathcal{Y}[[t]]$) that fix $t$ by the properties

i. $\Phi(x) = x(1-ty)^{-1}$

ii. $\Phi(x+y) = x + y$.

Proof. To characterize an automorphism $\Phi$ of $\mathcal{Y}[[t]]$ that fixes $t$, it is evidently enough to know where $\Phi$ sends $x$ and $y$; property (i) gives $\Phi(x)$, and then property (ii) gives $\Phi(y) = x + y - \Phi(x)$. To see that $\Phi = \bar{\sigma}_t\sigma_t^{-1}$ satisfies these properties, first note that

$$
\bar{\sigma}_t\sigma_t^{-1}(x) = \bar{\sigma}_t(E(-t)\cdot x) = \bar{\sigma}_t(x) = \tau\sigma_t(x) = \tau(H(t)\cdot y) =
$$

$$
\tau(y + th_1 \cdot y + t^2h_2 \cdot y + \cdots) = \tau(y + txy + t^2x^2y + \cdots) = x + txy + t^2xy^2 + \cdots,
$$

and then do a similar calculation to show that $\bar{\sigma}_t\sigma_t^{-1}(y) = y - txy(1-ty)^{-1}$. \quad \square

Now consider the derivation

$$
\partial_t = \sum_{n=1}^{\infty} t^n \frac{\partial_n}{n}
$$

of $\mathcal{Y}[[t]]$; by Lemma 5.7, $\exp(\partial_t)$ is an automorphism of $\mathcal{Y}[[t]]$. To show that $\partial_n(w) \in \ker \zeta$ for all $n \geq 1$ and $w \in \mathcal{Y}^0$ is equivalent to (13) (and thus to Theorem 5.6), it suffices to prove the following.
Theorem 5.9. \( \exp(\partial_t) = \bar{\sigma}_t \sigma_t^{-1} \).

Proof. We use Lemma 5.8. Since the derivations \( \partial_n \) all take \( z = x + y \) to 0, it is evident that \( \exp(\partial_t) \) satisfies property (ii). To show \( \exp(\partial_t)(x) = x(1 - ty)^{-1} \), set

\[
G(s) = \exp(s\partial_t)(x) = \sum_{n=0}^{\infty} \partial^n_t(x) \frac{s^n}{n!} \in \mathcal{H}[s, t].
\]

Then \( G(s) \) is the solution of the initial-value problem \( G'(s) = \partial_t G(s), G(0) = x \). We claim that

\[
G(s) = x \left( 1 - \frac{1 - (1 - tz)^s}{z} y \right)^{-1}
\]

since the right-hand side also satisfies these conditions; the conclusion then follows upon setting \( s = 1 \). To verify the claim, let \( U = (1 - (1 - tz)^s)/z \) and \( V = \log(1 - tz)/z \); then the right-hand side of equation (14) is

\[
x(1 - Uy)^{-1} = x(1 + Uy + UyUy + \cdots)
\]

and the claim follows from the identities \( U'(s) = UzV - V, \partial_t U = 0, \partial_t(x) = -xVy, \) and \( \partial_t(y) = zVy - yVy \).  

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