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Algebraic aspects of rooted tree maps

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Abstract
Based on the Connes–Kreimer Hopf algebra of rooted trees, rooted tree maps are defined as linear maps on the noncommutative polynomial algebra $\mathbb{Q}\langle x, y\rangle$. It is known that they induce a large class of linear relations for multiple zeta values. In this paper, we show for any rooted tree f there exists a unique polynomial in $\mathbb{Q}\langle x, y\rangle$ that gives the image of the rooted tree map $\tilde{f}$ explicitly. We also characterize the antipode maps as the conjugation by the special map τ.

Keywords Connes–Kreimer Hopf algebra of rooted trees · Rooted tree maps · Harmonic products · Multiple zeta values

Mathematics Subject Classification 05C05 · 16T05 · 11M32

1 Introduction

Let $\mathcal{H}$ be the Connes–Kreimer Hopf algebra of rooted trees introduced in [3]. For any $f \in \mathcal{H}$, the rooted tree map $\tilde{f}$ is introduced in [11] as an element in $\mathrm{End}(\mathcal{A})$, where $\mathcal{A}$ is the noncommutative polynomial algebra $\mathbb{Q}\langle x, y\rangle$. It is known that rooted tree maps induce a large class of linear relations for multiple zeta values. In [1, 2], we find some results in algebraic properties of rooted tree maps to make some applications to multiple zeta values clear. In [8], the quasi-derivation operator introduced in [7] can be

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interpreted by a certain kind of harmonic product $\diamond$ (introduced in [4]). In this paper, we establish similar algebraic formulas for rooted tree maps in the harmonic algebra.

Theorem 1.1 *For any $f \in \mathcal{H}$ and $w \in \mathcal{A}$, there exists a unique $F_f \in \mathcal{A}$ such that*

$$\tilde{f}(wx) = (F_f \diamond w)x.$$

Remark 1.2 The fact that rooted tree maps are commutative pairwisely, which is intricately shown in [T], follows immediately from our Theorem 1.1 because the product $\diamond$ is commutative. We call the rooted tree with n vertices among which there is only one leaf the ladder tree, which is denoted by λ_n. The corresponding rooted tree map $\widetilde{\lambda_n}$ is closely related to the derivation operator ∂_n, which gives the derivation relation for multiple zeta value's (see [BT] for details). On the other hand, one finds $F_{\lambda_n} = y(x+2y)^{n-1}$ (see Sect. 3). Combining these two, the derivation operator is expressed by the product $\diamond$. The expression agrees with Theorem 2.2 in [KMM] when $c = 0$. It's not been clear how the quasi-derivation operator relates to rooted tree maps, i.e., how our theorem 1.1 relates to Theorem 2.2 in [KMM] for arbitrary c.

We also have similar formulas for $\widetilde{S(f)} \in \mathrm{End}(\mathcal{A})$, where S denotes the antipode of $\mathcal{H}$.

Theorem 1.3 *For any $f \in \mathcal{H}$ and $w \in \mathcal{A}$, there exists a unique $G_f \in \mathcal{A}$ such that*

$$\widetilde{S(f)}(wx) = (G_f \diamond w)x.$$

By Theorems 1.1 and 1.3, we have $(G_f \diamond w)x = \widetilde{S(f)}(wx) = (F_{S(f)} \diamond w)x$ for $w \in \mathcal{A}$. Thus we obtain

Corollary 1.4 *For any $f \in \mathcal{H}$, we have*

$$G_f = F_{S(f)}.$$

Let τ be the anti-automorphism on $\mathcal{A}$ characterized by $\tau(x) = y$ and $\tau(y) = x$. This τ is an involution and gives the well-known duality formula for multiple zeta values. We also have the following property.

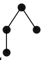
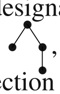
Theorem 1.5 *For any $f \in \mathcal{H}$, we have*

$$\widetilde{S(f)} = \tau \tilde{f} \tau.$$

In Sect. 2, we give some basic tools including the Connes–Kreimer Hopf algebra of rooted trees, rooted tree maps, and harmonic products. Sections 3–5 are devoted to Proofs of Theorems 1.1, 1.3, and 1.5 in turn.

2 Preliminaries

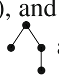
2.1 Connes–Kreimer Hopf algebra of rooted trees

We review briefly the Connes–Kreimer Hopf algebra of rooted trees introduced in [3]. A tree is a finite and connected graph without cycles and a rooted tree is a tree in which one vertex is designated as the root. We consider rooted trees without plane structure, e.g.,  $=$ , where the topmost vertex represents the root. A (rooted) forest is a finite collection of rooted trees $t_1, \dots, t_n$, which we denote by $t_1 \cdots t_n$. Then the Connes–Kreimer Hopf algebra of rooted trees $\mathcal{H}$ is the $\mathbb{Q}$-vector space freely generated by rooted forests with the commutative ring structure. We denote by $\mathbb{I}$ the empty forest, which is regarded as the neutral element in $\mathcal{H}$.

We define the linear map B_+ on $\mathcal{H}$ sending a forest $t_1 \cdots t_n$, where t_j's are trees, to the tree obtained by grafting all roots of t_j's onto a single vertex which is the new root, and $B_+(\mathbb{I}) = \bullet$. We find that, for a rooted tree $t (\neq \mathbb{I})$, there is a unique forest f such that $t = B_+(f)$. The coproduct Δ on $\mathcal{H}$ is defined by the following two rules.

(1) $\Delta(t) = \mathbb{I} \otimes t + (B_+ \otimes \mathrm{id}) \circ \Delta(f)$ if $t = B_+(f)$,
(2) $\Delta(f) = \Delta(g)\Delta(h)$ if $f = gh$ with $g, h \in \mathcal{H}$.

Note that components of the tensor product are reversely defined compared to those in [3]. We denote by S the antipode of $\mathcal{H}$. In the sequel, we often employ the Sweedler notation $\Delta(f) = \sum_{(f)} f' \otimes f''$.

A subtree t' of the rooted tree t (denoted by $t' \subset t$) is a subgraph of t that is connected and contains the root of t (hence the empty tree $\mathbb{I}$ cannot be a subtree in our sense), and we denote by $t \setminus t'$ their subtraction. For example, we have $t \setminus t' = \bullet$  if $t =$  and $t' = \bullet$.

Proposition 2.1 [3] *For a rooted tree t, we have*

(1) $\Delta(t) = \mathbb{I} \otimes t + \sum_{t' \subset t} t' \otimes (t \setminus t')$,

(2) $S(t) + \sum_{t' \subset t} t' S(t \setminus t') = 0$.

2.2 Rooted tree maps

We here define rooted tree maps introduced in [11]. For $u \in \mathcal{A}$, let L_u and R_u be $\mathbb{Q}$-linear maps on $\mathcal{A}$ defined by $L_u(w) = uw$ and $R_u(w) = wu$ $(w \in \mathcal{A})$. For $f \in \mathcal{H}$, we define the $\mathbb{Q}$-linear map $\tilde{f} \colon \mathcal{A} \to \mathcal{A}$, which we call the rooted tree map, recursively by

(1) $\tilde{\mathbb{I}} = \mathrm{id}$,
(2) $\tilde{f}(x) = yx$ and $\tilde{f}(y) = -yx$ if $f = \bullet$,
(3) $\tilde{t}(u) = L_y L_{x+2y} L_y^{-1} \tilde{f}(u)$ if $t = B_+(f)$,
(4) $\tilde{f}(u) = \tilde{g}(\tilde{h}(u))$ if $f = gh$,
(5) $\tilde{f}(uw) = \sum_{(f)} \widetilde{f'}(u)\widetilde{f''}(w)$ for $\Delta(f) = \sum_{(f)} f' \otimes f''$,

where $w \in \mathcal{A}$ and $u \in \{x, y\}$. It is known that $\widetilde{\ }: \mathcal{H} \to \mathrm{End}(\mathcal{A})$ is an algebra homomorphism. We sometimes denote its image by $\widetilde{\mathcal{H}}$. (Note that in this definition the order of the concatenation product on $\mathcal{A}$ is treated reversely compared to that in [11]. Since the coproduct Δ on $\mathcal{H}$ is also defined reversely as above, this definition makes sense.)

Let $z = x + y$. It is known that rooted tree maps commute with each other and with L_z and R_z.

Lemma 2.2 [11] *For $f \in \mathcal{H}$ and $w \in \mathcal{A}$, we have $\tilde{f}(zw) = z\tilde{f}(w)$ and $\tilde{f}(wz) = \tilde{f}(w)z$.*

2.3 Harmonic products

Let $\mathcal{A}^1 = \mathbb{Q} + y\mathcal{A}$ be a subalgebra of $\mathcal{A}$. We define the $\mathbb{Q}$-bilinear product $*$ on $\mathcal{A}^1$, which is called the harmonic product, by

$$\begin{aligned}
&w * 1 = 1 * w = w,\\
&yx^{k_1-1}\cdots yx^{k_r-1} * yx^{l_1-1}\cdots yx^{l_s-1}\\
&\quad = yx^{k_1-1}(yx^{k_2-1}\cdots yx^{k_r-1} * yx^{l_1-1}\cdots yx^{l_s-1})\\
&\qquad + yx^{l_1-1}(yx^{k_1-1}\cdots yx^{k_r-1} * yx^{l_2-1}\cdots yx^{l_s-1})\\
&\qquad + yx^{k_1+l_1-1}(yx^{k_2-1}\cdots yx^{k_r-1} * yx^{l_2-1}\cdots yx^{l_s-1}).
\end{aligned}$$

It is known that this product is commutative and associative, and has one of the product structures of multiple zeta values (see [5]). There are many properties of the harmonic product. We here recall the following identity (see [6, Proposition 6] or [9, Proposition 7.1]). For $yx^{k_1-1}\cdots yx^{k_r-1} \in \mathcal{A}^1$, we have

$$\sum_{i=0}^{r}(-1)^i yx^{k_1-1}\cdots yx^{k_i-1} * yx^{k_r-1}zx^{k_{r-1}-1}\cdots zx^{k_{i+1}-1} = 0. \tag{1}$$

Next, we define the $\mathbb{Q}$-bilinear product $\overline{*}$ on $\mathcal{A}^1$ by

$$\begin{aligned}
&w \,\overline{*}\, 1 = 1 \,\overline{*}\, w = w,\\
&yx^{k_1-1}\cdots yx^{k_r-1} \,\overline{*}\, yx^{l_1-1}\cdots yx^{l_s-1}\\
&\quad = yx^{k_1-1}(yx^{k_2-1}\cdots yx^{k_r-1} \,\overline{*}\, yx^{l_1-1}\cdots yx^{l_s-1})\\
&\qquad + yx^{l_1-1}(yx^{k_1-1}\cdots yx^{k_r-1} \,\overline{*}\, yx^{l_2-1}\cdots yx^{l_s-1})\\
&\qquad - yx^{k_1+l_1-1}(yx^{k_2-1}\cdots yx^{k_r-1} \,\overline{*}\, yx^{l_2-1}\cdots yx^{l_s-1}).
\end{aligned}$$

Let d_1 be the automorphism on $\mathcal{A}$ given by $d_1(x) = x$ and $d_1(y) = z$. We define the $\mathbb{Q}$-linear map $d\colon \mathcal{A}^1 \to \mathcal{A}^1$ by $d(1) = 1$ and $d(yw) = yd_1(w)$ for $w \in \mathcal{A}$. The map d intermediates between the two products in the following sense.

Lemma 2.3 [10] *For $w_1, w_2 \in \mathcal{A}^1$, we have*

$$d(w_1 \overline{*} w_2) = d(w_1) * d(w_2).$$

Lastly, following [4], we define the product $\diamond$ on $\mathcal{A}$ by

$$\begin{aligned} w \diamond 1 &= 1 \diamond w = w, \\ xw_1 \diamond xw_2 &= x(w_1 \diamond xw_2) - x(yw_1 \diamond w_2), \\ xw_1 \diamond yw_2 &= x(w_1 \diamond yw_2) + y(xw_1 \diamond w_2), \\ yw_1 \diamond xw_2 &= y(w_1 \diamond xw_2) + x(yw_1 \diamond w_2), \\ yw_1 \diamond yw_2 &= y(w_1 \diamond yw_2) - y(xw_1 \diamond w_2) \end{aligned} \tag{2}$$

for $w, w_1, w_2 \in \mathcal{A}$ together with $\mathbb{Q}$-bilinearity. We find that the product $\diamond$ is associative and commutative. Let ϕ be the automorphism on $\mathcal{A}$ given by $\phi(x) = z$ and $\phi(y) = -y$. We note that ϕ is an involution. The product $\diamond$ is thought of a kind of the harmonic product by virtue of $w_1 \diamond w_2 = \phi(\phi(w_1) * \phi(w_2))$ for $w_1, w_2 \in \mathcal{A}^1$.

Lemma 2.4 [4, Proposition 2.3] *For $w_1, w_2 \in \mathcal{A}$, we have*

$$zw_1 \diamond w_2 = w_1 \diamond zw_2 = z(w_1 \diamond w_2).$$

Lemma 2.5 *For $w_1, w_2 \in \mathcal{A}$, we have*

$$w_1xw_2 \diamond y = (w_1 \diamond y)xw_2 + w_1x(w_2 \diamond y).$$

Proof It is enough to consider the case that w_1 is a word. We prove the lemma by induction on $\deg(w_1)$. When $\deg(w_1) = 0$, we easily see the lemma holds.

Assume $\deg(w_1) \geq 1$. If $w_1 = zw_1'$ ($w_1' \in \mathcal{A}$), by the induction hypothesis and Lemma 2.4, we have

$$\mathrm{LHS} = z(w_1'xw_2 \diamond y) = z(w_1' \diamond y)xw_2 + zw_1'x(w_2 \diamond y) = \mathrm{RHS}.$$

If $w_1 = xw_1'$ ($w_1' \in \mathcal{A}$), by the induction hypothesis and (2), we have

$$\begin{aligned} \mathrm{LHS} &= x(w_1'xw_2 \diamond y) + yw_1xw_2 \\ &= x(w_1' \diamond y)xw_2 + w_1x(w_2 \diamond y) + yw_1xw_2 = \mathrm{RHS}. \end{aligned}$$

This finishes the proof. □

3 Proof of Theorem 1.1

In this section, we prove Theorem 1.1. For a forest f, we define the polynomial $F_f \in \mathcal{A}^1$ recursively by

(1) $F_{\mathbb{I}} = 1$,

(2) $F_\bullet = y$,
(3) $F_t = L_y L_{x+2y} L_y^{-1}(F_f)$ if $t = B_+(f)$ and $f \neq \mathbb{I}$,
(4) $F_f = F_g \diamond F_h$ if $f = gh$.

The subscript of F is extended linearly. Put $L = L_y L_{x+2y} L_y^{-1}$. To prove Theorem 1.1, next proposition plays a key role.

Proposition 3.1 *For $w_1, w_2 \in \mathcal{A}$ and $f \in \mathcal{H}$, we have*

$$w_1 x w_2 \diamond F_f = \sum_{(f)} (F_{f'} \diamond w_1) x (F_{f''} \diamond w_2),$$

where $\Delta(f) = \sum_{(f)} f' \otimes f''$.

Proof It is enough to consider the case that f is a forest. We prove the proposition by induction on $\deg(f)$.

When $\deg(f) = 1$, by Lemma 2.5, we find the proposition holds.

Assume $\deg(f) \geq 2$. If $f = gh$ $(g, h \neq \mathbb{I})$, by the induction hypothesis and the multiplicativity of the coproduct, we have

$$\begin{aligned}
w_1 x w_2 \diamond F_f &= w_1 x w_2 \diamond (F_g \diamond F_h)\\
&= (w_1 x w_2 \diamond F_g) \diamond F_h\\
&= \sum_{(g)} (F_{g'} \diamond w_1) x (F_{g''} \diamond w_2) \diamond F_h\\
&= \sum_{(g)} \sum_{(h)} (F_{h'} \diamond (F_{g'} \diamond w_1)) x (F_{h''} \diamond (F_{g''} \diamond w_2))\\
&= \sum_{(g)} \sum_{(h)} ((F_{h'} \diamond F_{g'}) \diamond w_1) x ((F_{h''} \diamond F_{g''}) \diamond w_2)\\
&= \sum_{(f)} (F_{f'} \diamond w_1) x (F_{f''} \diamond w_2).
\end{aligned}$$

If f is a tree (with $\deg(f) \geq 2$), we have $F_f = L(F_g)$, where $f = B_+(g)$.

In this case, we prove the statement for a word w_1 by induction on $\deg(w_1)$. When $\deg(w_1) = 0$, we have

$$\begin{aligned}
x w_2 \diamond F_f &= x w_2 \diamond L(F_g)\\
&= x w_2 \diamond y x L_y^{-1} F_g + x w_2 \diamond 2y F_g\\
&= x(w_2 \diamond y x L_y^{-1} F_g) + y(x w_2 \diamond x L_y^{-1} F_g) + x(w_2 \diamond 2y F_g)\\
&\quad + 2y(x w_2 \diamond F_g)\\
&= y(x w_2 \diamond x L_y^{-1} F_g) + x(w_2 \diamond L(F_g)) + 2y(x w_2 \diamond F_g).
\end{aligned}$$

For the last term on the right-hand side, we have

$$2y(x w_2 \diamond F_g) = 2 \sum_{(g)} y F_{g'} x (F_{g''} \diamond w_2) \qquad \text{(by induction)}$$

$$
\begin{aligned}
&= 2yx(F_g \diamond w_2) + 2\sum_{\substack{(g)\\ g'\neq \mathbb{I}}} yF_{g'}x(F_{g''} \diamond w_2)\\
&= 2yx(F_g \diamond w_2) + \sum_{\substack{(g)\\ g'\neq \mathbb{I}}} L(F_{g'})x(F_{g''} \diamond w_2)\\
&\quad - \sum_{\substack{(g)\\ g'\neq \mathbb{I}}} yxL_y^{-1}F_{g'}x(F_{g''} \diamond w_2).
\end{aligned}
$$

Then we find

$$
\begin{aligned}
xw_2 \diamond F_f = {} & y(xw_2 \diamond xL_y^{-1}F_g) + x(w_2 \diamond L(F_g)) + 2yx(F_g \diamond w_2)\\
& + \sum_{\substack{(g)\\ g'\neq \mathbb{I}}} L(F_{g'})x(F_{g''} \diamond w_2) - \sum_{\substack{(g)\\ g'\neq \mathbb{I}}} yxL_y^{-1}F_{g'}x(F_{g''} \diamond w_2).
\end{aligned}
$$

Since

$$
x(w_2 \diamond L(F_g)) + yx(F_g \diamond w_2) + \sum_{\substack{(g)\\ g'\neq \mathbb{I}}} L(F_{g'})x(F_{g''} \diamond w_2) = \sum_{(f)} F_{f'}x(F_{f''} \diamond w_2)
$$

(by Proposition 2.1(1) or the definition of Δ)

and

$$
\begin{aligned}
y(xw_2 \diamond xL_y^{-1}F_g) &= y(xL_y^{-1}F_g \diamond xw_2)\\
&= yx(L_y^{-1}F_g \diamond xw_2) - yx(F_g \diamond w_2),
\end{aligned}
$$

we have

$$
\begin{aligned}
xw_2 \diamond F_f = {} & \sum_{(f)} F_{f'}x(F_{f''} \diamond w_2) + yx(L_y^{-1}F_g \diamond xw_2)\\
& - \sum_{\substack{(g)\\ g'\neq \mathbb{I}}} yxL_y^{-1}F_{g'}x(F_{g''} \diamond w_2).
\end{aligned}
$$

Here we see

$$
L_y^{-1}F_g \diamond xw_2 = \sum_{(g)} L_y^{-1}F_{g'}x(F_{g''} \diamond w_2)
$$

since

$$
y(L_y^{-1}F_g \diamond xw_2) = yL_y^{-1}F_g \diamond xw_2 - x(w_2 \diamond F_g)
$$

$$
\begin{aligned}
&= F_g \diamond x w_2 - x(w_2 \diamond F_g) \\
&= \sum_{(g)} F_{g'} x(F_{g''} \diamond w_2) - x(w_2 \diamond F_g) \\
&= \sum_{\substack{(g) \\ g' \neq \mathbb{I}}} F_{g'} x(F_{g''} \diamond w_2).
\end{aligned}
$$

Hence we get

$$
x w_2 \diamond F_f = \sum_{(f)} F_{f'} x(F_{f''} \diamond w_2).
$$

Now we proceed to the case when $\deg(w_1) \geq 1$.
If $w_1 = z w_1'$ ($w_1' \in \mathcal{A}$), we have

$$
\begin{aligned}
z w_1' x w_2 \diamond F_f &= z(w_1' x w_2 \diamond F_f) \\
&= z \sum_{(f)} (F_{f'} \diamond w_1') x(F_{f''} \diamond w_2) \\
&= \sum_{(f)} (F_{f'} \diamond w_1) x(F_{f''} \diamond w_2)
\end{aligned}
$$

by the induction hypothesis.
If $w_1 = x w_1'$ ($w_1' \in \mathcal{A}$), since we have already proved the identity in the case of $w_1 = 1$, we have

$$
\begin{aligned}
w_1 x w_2 \diamond F_f &= \sum_{(f)} F_{f'} x(F_{f''} \diamond w_1' x w_2) \\
&= \sum_{(f)} F_{f'} x \sum_{(f'')} (F_{f_a''} \diamond w_1') x(F_{f_b''} \diamond w_2),
\end{aligned}
$$

where we put $\Delta(f'') = \sum_{(f'')} f_a'' \otimes f_b''$.
We also have

$$
\begin{aligned}
\sum_{(f)} (F_{f'} \diamond w_1) x(F_{f''} \diamond w_2) &= \sum_{(f)} (F_{f'} \diamond x w_1') x(F_{f''} \diamond w_2) \\
&= \sum_{(f)} \sum_{(f')} F_{f_a'} x(F_{f_b'} \diamond w_1') x(F_{f''} \diamond w_2),
\end{aligned}
$$

where we put $\Delta(f') = \sum_{(f')} f_a' \otimes f_b'$.
By the coassociativity of Δ, we find the result. □

Proof of Theorem 1.1 We prove the theorem only for forests f and words w by induction on $\deg(f)$ and $\deg(w)$. Note that the existence and the uniqueness of $F_f \in \mathcal{A}$

can also be confirmed by following the proof. First, we prove the theorem when $\deg(f) = 1$.

If $\deg(w) = 0$, we easily find the result.

Suppose $\deg(w) \geq 1$. If $w = zw'$ $(w' \in \mathcal{A})$, by Lemmas 2.2 and 2.4, and the induction hypothesis, we have

$$\mathrm{LHS} = \tilde{f}(zw'x) = z\tilde{f}(w'x) = z(F_f \diamond w')x = (F_f \diamond zw')x = \mathrm{RHS}.$$

On the other hand, if $w = xw'$ $(w' \in \mathcal{A})$, we have

$$\mathrm{LHS} = \tilde{f}(xw'x) = yxw'x + x\tilde{f}(w'x)$$

and

$$\mathrm{RHS} = (y \diamond xw')x = yxw'x + x(y \diamond w')x.$$

By the induction hypothesis, we find the result.

Next, suppose $\deg(f) \geq 2$. If $f = gh$ $(g, h \neq \mathbb{I})$, we have

$$\begin{aligned}
&\tilde{f}(wx) \\
&\quad = \tilde{g}\tilde{h}(wx) = \tilde{g}((F_h \diamond w)x) = (F_g \diamond (F_h \diamond w))x \\
&\quad = ((F_g \diamond F_h) \diamond w)x = (F_f \diamond w)x.
\end{aligned}$$

Let f be a rooted tree and put $f = B_+(g)$.

When $\deg(w) = 0$, we have

$$\tilde{f}(x) = (yxL_y^{-1} + 2y)\tilde{g}(x) = (yxL_y^{-1} + 2y)F_g x = F_f x.$$

Suppose $\deg(w) \geq 1$. If $w = zw'$ $(w' \in \mathcal{A})$, we have

$$\tilde{f}(zw'x) = z\tilde{f}(w'x) = z(F_f \diamond w')x = (F_f \diamond zw')x$$

by Lemmas 2.2 and 2.4.

If $w = xw'$ $(w' \in \mathcal{A})$, we have

$$\tilde{f}(xw'x) = \sum_{(f)} \widetilde{f'}(x)\widetilde{f''}(w'x) = \sum_{(f)} F_{f'}x(F_{f''} \diamond w')x$$

by the induction hypothesis.

By Proposition 3.1, we have

$$(F_f \diamond xw')x = \sum_{(f)} F_{f'}x(F_{f''} \diamond w')x.$$

This completes the proof. $\square$

4 Proof of Theorem 1.3

Let $\mathcal{A}^1_*$ be the commutative $\mathbb{Q}$-algebra with the harmonic product $*$. We define the $\mathbb{Q}$-linear map $u\colon \mathcal{A} \to \mathcal{A}^* \otimes \mathcal{A}^*$ by $u(1) = 1$ and sending a word $w = yx^{k_1-1} \cdots yx^{k_r-1}$ to

$$\sum_{i=0}^{r}(-1)^i yx^{k_1-1} \cdots yx^{k_i-1} \otimes yx^{k_r-1}zx^{k_{r-1}-1} \cdots zx^{k_{i+1}-1}.$$

The notation u_w is sometimes used instead of $u(w)$ for convenience. Let $\mathcal{B} \subset \mathcal{A}^1_* \otimes \mathcal{A}^1_*$ be the $\mathbb{Q}$-subalgebra algebraically generated by u_w's. The product of the tensor algebra is given component wisely so that

$$\begin{aligned} &u(yx^{k_1-1} \cdots yx^{k_r-1}) * u(yx^{l_1-1} \cdots yx^{l_s-1}) \\ &= \sum_{i=0}^{r}\sum_{j=0}^{s}(-1)^{i+j}(yx^{k_1-1} \cdots yx^{k_i-1} * yx^{l_1-1} \cdots yx^{l_j-1}) \\ &\qquad \otimes (yx^{k_r-1}zx^{k_{r-1}-1} \cdots zx^{k_{i+1}-1} * yx^{l_s-1}zx^{l_{s-1}-1} \cdots zx^{l_{j+1}-1}). \end{aligned}$$

Now we define the $\mathbb{Q}$-linear map $\rho\colon\ y\mathcal{A} \to y\mathcal{A}$ by setting $\rho(1) = 1$ and $\rho = L_y \epsilon L_y^{-1}$, where ϵ is the anti-automorphism on $\mathcal{A}$ such that $\epsilon(x) = x$ and $\epsilon(y) = y$. Note that $\rho(yx^{k_1-1} \cdots yx^{k_r-1}) = yx^{k_r-1} \cdots yx^{k_1-1}$. Put $L'_a(w_1 \otimes w_2) = yx^{a-1}w_1 \otimes w_2$ for $a \in \mathbb{Z}_{\geq 1}$.

Lemma 4.1 *For $w_1, w_2 \in \mathcal{A}^1$, we have*

$$u(w_1 \mathbin{\overline{*}} w_2) = u(w_1) * u(w_2).$$

Proof It is enough to show the lemma for $w_1 = yx^{k_1-1} \cdots yx^{k_r-1}$ and $w_2 = yx^{l_1-1} \cdots yx^{l_s-1}$. The proof goes by induction on $r + s$. The lemma holds when $r + s \leq 1$ since $u(1) = 1 \otimes 1$. Assume $r + s \geq 2$. Note that

$$\begin{aligned} u(w) &= 1 \otimes yx^{m_t-1}zx^{m_{t-1}-1} \cdots zx^{m_1-1} - L'_{m_1}u(yx^{m_2-1} \cdots yx^{m_t-1}) \\ &= 1 \otimes d\rho(w) - L'_{m_1}u(yx^{m_2-1} \cdots yx^{m_t-1}) \end{aligned} \tag{3}$$

holds for $w = yx^{m_1-1} \cdots yx^{m_t-1}$. By definitions and the induction hypothesis, we have

$$\begin{aligned} &u(w_1 \mathbin{\overline{*}} w_2) \\ &= u(yx^{k_1-1}(yx^{k_2-1} \cdots yx^{k_r-1} \mathbin{\overline{*}} w_2) + yx^{l_1-1}(w_1 \mathbin{\overline{*}} yx^{l_2-1} \cdots yx^{l_s-1}) \\ &\qquad - yx^{k_1+l_1-1}(yx^{k_2-1} \cdots yx^{k_r-1} \mathbin{\overline{*}} yx^{l_2-1} \cdots yx^{l_s-1})) \\ &= 1 \otimes d\rho(w_1 \mathbin{\overline{*}} w_2) - L'_{k_1}(u(yx^{k_2-1} \cdots yx^{k_r-1}) * u(w_2)) \\ &\quad + 1 \otimes d\rho(w_1 \mathbin{\overline{*}} w_2) - L'_{l_1}(u(w_1) * u(yx^{l_2-1} \cdots yx^{l_s-1})) \end{aligned}$$

$$
\begin{aligned}
&- 1 \otimes d\rho(w_1 \mathbin{\overline{*}} w_2) \\
&+ L'_{k_1+l_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(yx^{l_2-1}\cdots yx^{l_s-1})) \qquad \text{(by (3))} \\
&= 1 \otimes d\rho(w_1 \mathbin{\overline{*}} w_2) - L'_{k_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(w_2)) \\
&- L'_{l_1}(u(w_1) * u(yx^{l_2-1}\cdots yx^{l_s-1})) \\
&+ L'_{k_1+l_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(yx^{l_2-1}\cdots yx^{l_s-1}))
\end{aligned}
$$

and

$$
\begin{aligned}
&u(w_1) * u(w_2) \\
&= (1 \otimes d\rho(w_1) - L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1})) * (1 \otimes d\rho(w_2) \\
&\quad - L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1})) \\
&= 1 \otimes (d\rho(w_1) * d\rho(w_2)) - L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1}) * (1 \otimes d\rho(w_2)) \\
&\quad - (1 \otimes d\rho(w_1)) * L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1}) \\
&\quad + L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1}) * L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1}).
\end{aligned}
$$

Let us show that these two coincide. Because of Lemma 2.3 and $\rho(w_1 \mathbin{\overline{*}} w_2) = \rho(w_1) \mathbin{\overline{*}} \rho(w_2)$, we have

$$
d\rho(w_1 \mathbin{\overline{*}} w_2) = d\rho(w_1) * d\rho(w_2).
$$

Also we find that

$$
\begin{aligned}
&- L'_{k_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(w_2)) + L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1}) * (1 \otimes d\rho(w_2)) \\
&= -L'_{k_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(w_2) - u(yx^{k_2-1}\cdots yx^{k_r-1}) * (1 \otimes d\rho(w_2))) \\
&= -L'_{k_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1}))
\end{aligned}
$$

and

$$
\begin{aligned}
&- L'_{l_1}(u(w_1) * u(yx^{l_2-1}\cdots yx^{l_s-1})) + (1 \otimes d\rho(w_1)) * L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1}) \\
&= -L'_{l_1}(u(w_1) * u(yx^{l_2-1}\cdots yx^{l_s-1}) - (1 \otimes d\rho(w_1)) * u(yx^{l_2-1}\cdots yx^{l_s-1})) \\
&= -L'_{l_1}(L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(yx^{l_2-1}\cdots yx^{l_s-1})).
\end{aligned}
$$

Since

$$
\begin{aligned}
&L'_{k_1+l_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(yx^{l_2-1}\cdots yx^{l_s-1})) \\
&- L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1}) * L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1}) \\
&= L'_{k_1}(u(yx^{k_2-1}\cdots yx^{k_r-1}) * L'_{l_1}u(yx^{l_2-1}\cdots yx^{l_s-1})) \\
&\quad + L'_{l_1}(L'_{k_1}u(yx^{k_2-1}\cdots yx^{k_r-1}) * u(yx^{l_2-1}\cdots yx^{l_s-1})),
\end{aligned}
$$

we have the result. □

Write $u_w = \sum_{i=0}^{r} u'_{w,i} \otimes u''_{w,i} = \sum_w u'_w \otimes u''_w$. We define the $\mathbb{Q}$-linear maps $p, q \colon \mathcal{B} \to \mathcal{A}^* \otimes \mathcal{A}^*$ by

$$\begin{aligned} p(u_{w_1} * \cdots * u_{w_r}) &= \sum_{\substack{u'_{w_1} \cdots u'_{w_r} \notin \mathbb{Q} \\ w_1,\ldots,w_r}} yxL_y^{-1}(u'_{w_1} * \cdots * u'_{w_r}) \otimes (u''_{w_1} * \cdots * u''_{w_r}) \\ &\quad + 1 \otimes (d\rho(w_1) * \cdots * d\rho(w_1))x, \\ q(u_{w_1} * \cdots * u_{w_r}) &= \sum_{w_1,\ldots,w_r} y(u'_{w_1} * \cdots * u'_{w_r}) \otimes (u''_{w_1} * \cdots * u''_{w_r}) \\ &\quad - 1 \otimes (d\rho(w_1) * \cdots * d\rho(w_1))z. \end{aligned}$$

Lemma 4.2 *We have* Im p, Im $q \subset \mathcal{B}$.

Proof From Lemma 4.1, we have

$$u_{w_1} * \cdots * u_{w_r} = u(w_1 \mathbin{\overline{*}} \cdots \mathbin{\overline{*}} w_r).$$

Thus, we need only to prove the lemma for the case $r = 1$. Since

$$p(u_w) = 1 \otimes d\rho(w)x + \sum_w yxL_y^{-1}u'_w \otimes u''_w = u(yx^{k_1}yx^{k_2-1} \cdots yx^{k_r-1}) \in \mathcal{B},$$

$$q(u_w) = L'_y(u_w) - 1 \otimes d\rho(w)z = u(y^2x^{k_1-1}yx^{k_2-1} \cdots yx^{k_r-1}) \in \mathcal{B},$$

we obtain the result. □

For a forest f, we define the polynomial $G_f \in \mathcal{A}^1$ recursively by

(1) $G_{\mathbb{I}} = 1$,
(2) $G_{\bullet} = -y$,
(3) $G_t = R_{2x+y}(G_f)$ if $t = B_+(f)$ and $f \neq \mathbb{I}$,
(4) $G_f = G_g \diamond G_h$ if $f = gh$.

The subscript of G is extended linearly. The following lemma is immediate from Lemmas 4.1 and 4.2, and definitions.

Lemma 4.3 *Let f be any forest with $f \neq \mathbb{I}$. If $\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''}) \in \mathcal{B}$, we have*

$$p\left(\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''})\right) = \sum_{\substack{(f) \\ f' \neq \mathbb{I}}} yxL_y^{-1}\phi(F_{f'}) \otimes \phi(G_{f''}) + \phi(F_{\mathbb{I}}) \otimes \phi(G_f)x \in \mathcal{B},$$

$$\begin{aligned} q\left(\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''})\right) &= \sum_{\substack{(f) \\ f' \neq \mathbb{I}}} y\phi(F_{f'}) \otimes \phi(G_{f''}) + y\phi(F_{\mathbb{I}}) \otimes \phi(G_f) \\ &\quad - \phi(F_{\mathbb{I}}) \otimes \phi(G_f)z \in \mathcal{B}. \end{aligned}$$

Proposition 4.4 *For any forest $f \neq \mathbb{I}$, we have*

$$\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''}) \in \mathcal{B}.$$

Proof We prove the proposition by induction on $\deg(f)$. When $\deg(f) = 1$, we easily see the statement holds.

Assume $\deg(f) \geq 2$. If $f = gh\ (g, h \neq \mathbb{I})$, since $\phi(F_g \diamond F_h) = \phi(F_g) * \phi(F_h)$, we have

$$\begin{aligned}\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''}) &= \sum_{\substack{(g)\\(h)}} \phi(F_{g'} \diamond F_{h'}) \otimes \phi(F_{g''} \diamond F_{h''}) \\ &= \sum_{(g)} \sum_{(h)} \big(\phi(F_{g'}) \otimes \phi(G_{g''})\big) * (\phi(F_{h'}) \otimes \phi(G_{h''}))\,.\end{aligned}$$

By the induction hypothesis, we find the result.

If f is a tree, we put $f = B_+(g)$.

Since

$$\Delta(f) = \mathbb{I} \otimes f + (B_+ \otimes \mathrm{id})\Delta(g),$$

we have

$$\begin{aligned}&\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''}) \\ &\quad = \phi(F_{\mathbb{I}}) \otimes \phi(G_{B_+(g)}) + \sum_{(g)} \phi(F_{B_+(g')}) \otimes \phi(G_{g''}) \\ &\quad = \phi(F_{\mathbb{I}}) \otimes \phi(G_g(2x+y)) \\ &\qquad + \sum_{\substack{(g)\\ g' \neq \mathbb{I}}} \phi((yxL_y^{-1} + 2y)F_{g'}) \otimes \phi(G_{g''}) + \phi(yF_{\mathbb{I}}) \otimes \phi(G_g) \\ &\quad = \sum_{\substack{(g)\\ g' \neq \mathbb{I}}} (yzL_y^{-1} - 2y)\phi(F_{g'}) \otimes \phi(G_{g''}) \\ &\qquad - y\phi(F_{\mathbb{I}}) \otimes \phi(G_g) + \phi(F_{\mathbb{I}}) \otimes \phi(G_g)(x+z).\end{aligned}$$

Then we get

$$\sum_{(f)} \phi(F_{f'}) \otimes \phi(G_{f''}) = (p-q)\Bigg(\sum_{(g)} \phi(F_{g'}) \otimes \phi(G_{g''})\Bigg).$$

By the induction hypothesis, we have $\sum_{(g)} \phi(F_{g'}) \otimes \phi(G_{g''}) \in \mathcal{B}$. Then, by Lemma 4.3, we find the result. ◻

Let $\mathrm{Aug} = \bigoplus_{n\geq 1} \mathcal{H}_n$ be the augmentation ideal, where $\mathcal{H}_n$ is the degree n homogeneous part of $\mathcal{H}$. We define the $\mathbb{Q}$-linear map $M\colon \mathcal{A}^1_* \otimes \mathcal{A}^1_* \to \mathcal{A}^1_*$ by $M(w_1 \otimes w_2) = w_1 * w_2$. Note that $M(w) = 0$ for $w \in \mathcal{B}$ by (1) in Sect. 2.3.

Proposition 4.5 *For any* $f \in \mathrm{Aug}$, *we have*

$$\sum_{(f)} F_{f'} \diamond G_{f''} = 0.$$

Proof We note that $\phi(w_1) * \phi(w_2) = \phi(w_1 \diamond w_2)$ holds for $w_1, w_2 \in \mathcal{A}$. By Proposition 4.4, we have

$$0 = \sum_{(f)} M(\phi(F_{f'}) \otimes \phi(G_{f''})) = \sum_{(f)} \phi(F_{f'} \diamond G_{f''}).$$

Then we find the result. □

Proof of Theorem 1.3 We prove the theorem by induction on $\deg(f)$. Note that the existence and the uniqueness of $G_f \in \mathcal{A}$ can also be confirmed by following the proof. It is easy to see the theorem holds if $\deg(f) = 1$. Suppose $\deg(f) \geq 2$. If $f = gh$ $(g, h \neq \mathbb{I})$, we have

$$\begin{aligned}
\widetilde{S(f)}(wx) = \widetilde{S(gh)}(wx) = \widetilde{S(g)}((G_h \diamond w)x)
&= (G_g \diamond (G_h \diamond w))x \\
&= ((G_g \diamond G_h) \diamond w)x \\
&= (G_f \diamond w)x.
\end{aligned}$$

If $f = t$ is a tree, by Proposition 4.5, Theorem 1.1, and the induction hypothesis, we have

$$\begin{aligned}
(G_t \diamond w)x &= -\sum_{t' \subset t} ((F_{t'} \diamond G_{t \setminus t'}) \diamond w)x \\
&= -\sum_{t' \subset t} (F_{t'} \diamond (G_{t \setminus t'} \diamond w))x \\
&= -\sum_{t' \subset t} \tilde{t'}((G_{t \setminus t'} \diamond w)x) \\
&= -\sum_{t' \subset t} \tilde{t'} \widetilde{S(t \setminus t')}(wx).
\end{aligned}$$

Since $\widetilde{S(t)} + \sum_{t' \subset t} \tilde{t'} \widetilde{S(t \setminus t')} = 0$ by Proposition 2.1 (2), we have

$$(G_t \diamond w)x = \widetilde{S(t)}(wx).$$

□

5 Proof of Theorem 1.5

Proof of Theorem 1.5 First, we prove the theorem when $w \in y\mathcal{A}x$. Put $w = yw'x$. By Theorem 1.3 and Corollary 1.4, we have

$$\widetilde{S(f)}(w) = (F_{S(f)} \diamond yw')x.$$

We also have

$$\begin{aligned}\tau\tilde{f}\tau(w) &= \tau\tilde{f}(y\tau(w')x)\\ &= \tau((F_f \diamond y\tau(w'))x) \qquad \text{(by Theorem 1.1)}\\ &= -\tau((y\tau L_y^{-1}(F_{S(f)}) \diamond y\tau(w'))x) \qquad \text{(by Proposition 5.1)}\\ &= -y\tau(y\tau L_y^{-1}(F_{S(f)}) \diamond y\tau(w'))\\ &= (F_{S(f)} \diamond yw')x \qquad \text{(by Lemma 5.2)}.\end{aligned}$$

Thus we have

$$\widetilde{S(f)}(w) = \tau\tilde{f}\tau(w) \tag{4}$$

for $w \in y\mathcal{A}x$.

Next, we prove the theorem when $w \in z\mathcal{A}x$ by induction on $\deg(w)$. Put $w = zw'x$. Then, by Lemma 2.2, we have

$$\begin{aligned}\widetilde{S(f)}(w) &= z\widetilde{S(f)}(w'x),\\ \tau\tilde{f}\tau(w) &= \tau\tilde{f}\tau(zw'x) = z\tau\tilde{f}\tau(w'x).\end{aligned}$$

By (4) and the induction hypothesis, we have

$$\widetilde{S(f)}(w'x) = \tau\tilde{f}\tau(w'x) \tag{5}$$

for any $w' \in \mathcal{A}$, and hence the assertion.

Finally, we prove the theorem when $w \in \mathcal{A}z$ by induction on $\deg(w)$. Put $w = w'z$. Then we have

$$\begin{aligned}\widetilde{S(f)}(w) &= (\widetilde{S(f)}(w'))z,\\ \tau\tilde{f}\tau(w) &= \tau\tilde{f}\tau(w'z) = (\tau\tilde{f}\tau(w'))z.\end{aligned}$$

By the induction hypothesis and (5), we have the assertion. Therefore we have $\widetilde{S(f)}(w) = \tau\tilde{f}\tau(w)$ for any $w \in \mathcal{A}$. □

Proposition 5.1 *For* $f \in \mathrm{Aug}$, *we have*

$$F_f = -y\tau L_y^{-1} F_{S(f)}.$$

Proof It is sufficient to prove the proposition for forests f by induction on $\deg(f)$. Since $F_\bullet = y$ and $F_{S(\bullet)} = -y$, the proposition hols for $\deg(f) = 1$.

Suppose $\deg(f) \geq 2$. If $f = gh$ $(g, h \neq \mathbb{I})$, we have

$$\begin{aligned} F_f &= F_g \diamond F_h \\ &= y\tau L_y^{-1}(G_g) \diamond y\tau L_y^{-1}(G_h) \qquad \text{(by induction and Corollary 1.4)} \\ &= -R_x^{-1}\tau((G_g \diamond G_h)x) \qquad \text{(by Lemma 5.2)} \end{aligned}$$

and

$$y\tau L_y^{-1} G_f = y\tau L_y^{-1}(G_g \diamond G_h) = R_x^{-1}\tau((G_g \diamond G_h)x).$$

Thus we have the result.

If f is a tree, put $f = B_+(g)$. Then we have

$$\begin{aligned} F_f &= L(F_g) \\ &= -L(y\tau L_y^{-1} G_g) \qquad \text{(by induction and Corollary 1.4)} \\ &= -y(x+2y)R_x^{-1}\tau(G_g) \end{aligned}$$

and

$$-y\tau L_y^{-1} G_f = -y\tau L_y^{-1} R_{2x+y}(G_g) = -y(x+2y)R_x^{-1}\tau(G_g).$$

This finishes the proof. □

Now we define $\sigma \in \mathrm{Aut}(\mathcal{A})$ such that $\sigma(x) = x$ and $\sigma(y) = -y$. By definitions, we have

$$-\phi R_x^{-1}\tau R_x \phi = d\rho\sigma. \tag{6}$$

We find that $d\sigma$ and ρ are homomorphisms with respect to the harmonic product $*$, and ρ commutes with σ. Hence the composition $d\rho\sigma$ is also a homomorphism with respect to the harmonic product $*$, and so is $-\phi R_x^{-1}\tau R_x \phi$ because of (6). This implies the composition $-R_x^{-1}\tau R_x$ is a homomorphism with respect to the product $\diamond$ (defined in Sect. 2) and hence we conclude the following lemma.

Lemma 5.2 *For $w_1, w_2 \in \mathcal{A}$, we have*

$$(yw_1 \diamond yw_2)x + y\tau(y\tau(w_1) \diamond y\tau(w_2)) = 0.$$

Proof We have

$$\begin{aligned} yw_1 \diamond yw_2 &= R_x^{-1} L_y(w_1 x) \diamond R_x^{-1} L_y(w_2 x) \\ &= R_x^{-1}\tau R_x \tau(w_1 x) \diamond R_x^{-1}\tau R_x \tau(w_2 x) \end{aligned}$$

$$= -R_x^{-1}\tau R_x(w_1x \diamond w_2x).$$

This gives the lemma. □

Remark 5.1 According to [2], for any $w \in y\mathcal{A}x$, there exists $\tilde{f} \in \widetilde{\mathcal{H}}$ such that $w = \tilde{f}(x)$. Hence we have $(1-\tau)(w) = (1-\tau)(\tilde{f}(x)) = (\tilde{f}+\tau\tilde{f}\tau)(x) = (\tilde{f}+\widetilde{S(f)})(x)$ due to Theorem 1.5, which means each of the duality formulas for multiple zeta values also appears in this form in the context of rooted tree maps.

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