Derivation relations and regularized double shuffle relations of multiple zeta values

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Abstract

Two kinds of linear relations of multiple zeta values, the derivation relations and the regularized double shuffle relations, are proved. Also presented is a conjectural formula which implies that the derivation relations are contained in the regularized double shuffle relations. A "formal KZ associator" is defined and is discussed briefly.

1 Introduction

We shall study linear relations of multiple zeta values in an algebraic setup. Following Hoffman [2], we let $\mathfrak{h} = \mathbf{Q}\langle x, y\rangle$ be the non-commutative polynomial algebra over the rationals in two indeterminates x and y, $\mathfrak{h}^1$ and $\mathfrak{h}^0$ its subalgebras $\mathbf{Q}+\mathfrak{h}y$ and $\mathbf{Q}+x\mathfrak{h}y$ respectively. Let $\widehat{\zeta}: \mathfrak{h}^0 \to \mathbf{R}$ be the $\mathbf{Q}$-linear map which assigns each monomial (word) $u_1u_2\cdots u_k$ in $\mathfrak{h}^0$ the multiple integral

$$\int\cdots\int_{1>t_1>t_2>\cdots>t_k>0} \frac{dt_1}{A_1(t_1)}\frac{dt_2}{A_2(t_2)}\cdots\frac{dt_k}{A_k(t_k)} \tag{1}$$

where $A_i(t)$ stands for t or $1-t$ according as u_i is x or y. We set $\widehat{\zeta}(1)=1$. Since the word $u_1u_2\cdots u_k$ is in $\mathfrak{h}^0$, we always have $A_1(t)=t$ and $A_k(t)=1-t$, hence the integral converges. In different terms, $\widehat{\zeta}$ is the $\mathbf{Q}$-linear map from $\mathfrak{h}^0$ to $\mathbf{R}$ characterized by $\widehat{\zeta}(1)=1$ and $\widehat{\zeta}(x^{k_1-1}yx^{k_2-1}y\cdots x^{k_n-1}y) = \zeta(k_1,k_2,\ldots,k_n)$ for $k_i\in\mathbf{N}$, $k_1>1$, where

$$\zeta(k_1,k_2,\ldots,k_n) = \sum_{\substack{m_1>m_2>\cdots>m_n>0\\ m_i\in\mathbf{Z}}} \frac{1}{m_1^{k_1}m_2^{k_2}\cdots m_n^{k_n}} \tag{2}$$

is the multiple zeta value (abbreviated to MZV). The weight $k=k_1+k_2+\cdots+k_n$ of $\zeta(k_1,k_2,\ldots,k_n)$ is the total degree of the corresponding monomial $x^{k_1-1}yx^{k_2-1}y\cdots x^{k_n-1}y$ and the depth n the degree in y. The first index k_1 in the index set $(k_1,k_2,\ldots,k_n)$ that corresponds to a word in $\mathfrak{h}^0$ is necessarily greater than 1, which ensures the convergence of the series in (2). The index set with this condition is referred later to as "admissible". The correspondence between the index set $(k_1,k_2,\ldots,k_n)$ of a MZV (2) and the integrand in (1) is given as follows. The dimension k of the integral is equal to the weight $k=k_1+k_2+\cdots+k_n$. If $i\in\{k_1,k_1+k_2,\ldots,k_1+k_2+\cdots+k_n\}$, then $A_i(t)=1-t$ and $A_i(t)=t$ otherwise.

Having defined the map $\widehat{\zeta}$, one of the fundamental problems in the theory of multiple zeta values is stated as

Problem: What is $\operatorname{Ker}\widehat{\zeta}$?

Producing elements of $\operatorname{Ker}\widehat{\zeta}$ amounts to finding linear relations among MZVs. In this paper, we shall discuss two methods of supplying elements in $\operatorname{Ker}\widehat{\zeta}$, the derivation relations and the regularized double shuffle relations, and their (conjectural) relationship.

In §2 we state and prove the derivation relations (Theorem 4). In §3, after the introduction of the regularization map, the regularized double shuffle relations (Theorem 9) will be formulated and proved. The proof uses Don Zagier's theorem on a relation between two kinds of re-normalization of divergent multiple zeta values. In §4, a reinterpretation of the regularization map in terms of certain derivations is given. A conjecture on a relation between the derivation relations and the regularized double shuffle relations will be stated in §5, with some results supporting the conjecture. In the final section §6, we define a "formal KZ associator" and discuss its properties and related problems.

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2 Derivation relations

Let $\operatorname{Der}(\mathfrak{h})$ be the Lie algebra of derivations (with respect to the concatenation product, Lie algebra structure being defined by $[\partial, \partial'] := \partial\partial' - \partial'\partial$ as usual) of $\mathfrak{h}$. Clearly, an element of $\operatorname{Der}(\mathfrak{h})$ is uniquely determined by the images of x and y.

Let $\tau : \mathfrak{h} \to \mathfrak{h}$ be the involutory anti-homomorphism which interchanges x and y. The involution τ preserves $\mathfrak{h}^0$, and the standard duality theorem for MZVs is the following.

Theorem 1 (Duality) *For any $w_0 \in \mathfrak{h}^0$, we have $(1-\tau)(w_0) \in \operatorname{Ker}\widehat{\zeta}$.*

Inspired by [4], we define the following elements $\partial_n \in \operatorname{Der}(\mathfrak{h})$.

Definition 2 *For $n \geq 1$, let $\partial_n \in \operatorname{Der}(\mathfrak{h})$ be defined by $\partial_n(x) = x(x+y)^{n-1}y$ and $\partial_n(y) = -x(x+y)^{n-1}y$.*

Obviously we have $\partial_n(\mathfrak{h}^0) \subset \mathfrak{h}^0$.

Lemma 3 $[\partial_m, \partial_n] = 0, \forall m, n \geq 1$.

Proof. Since $\partial_m(x+y) = 0$ for all m, it is enough to check that $\partial_m\partial_n(x) = \partial_n\partial_m(x)$.

Also note that $\partial_m((x+y)^k) = 0$ for all m and k. Using this,

$$\begin{aligned}
\partial_m\partial_n(x) &= \partial_m(x(x+y)^{n-1}y) \\
&= x(x+y)^{m-1}y(x+y)^{n-1}y - x(x+y)^{n-1}x(x+y)^{m-1}y \\
&= x(x+y)^{m-1}(x+y-x)(x+y)^{n-1}y \\
&\quad -x(x+y)^{n-1}(x+y-y)(x+y)^{m-1}y \\
&= -x(x+y)^{m-1}x(x+y)^{n-1}y + x(x+y)^{n-1}y(x+y)^{m-1}y \\
&= \partial_n\partial_m(x).
\end{aligned}$$

∎

Theorem 4 *For all $n \geq 1$ and $w_0 \in \mathfrak{h}^0$, we have $\partial_n(w_0) \in \operatorname{Ker}\widehat{\zeta}$.*

The case when $n = 1$ is equivalent to Hoffman's reformulation [4] of his previous theorem [3]. We deduce the theorem from Ohno's relation [7] (which simultaneously generalize duality, sum formula, and Hoffman's relations).

First, we introduce yet other derivations. For each integer $m \geq 1$, we define an element $D_m \in \operatorname{Der}(\mathfrak{h})$ by $D_m(x) = 0$ and $D_m(y) = x^m y$. Note that D_m's commute with each other: $[D_m, D_n] = 0$. Put $\overline{D}_m = \tau D_m \tau$. It is readily checked that $\overline{D}_m$ is again a derivation which sends x to xy^m and y to 0, and $[\overline{D}_m, \overline{D}_n] = 0$.

We shall work in the completion $\widehat{\mathfrak{h}} := \mathbf{Q}\langle\langle x, y\rangle\rangle$ of $\mathfrak{h}$, the non-commutative formal power series algebra over $\mathbf{Q}$. (Anti-)homomorphisms and derivations of $\mathfrak{h}$ such as τ or ∂_n naturally extend to those of $\widehat{\mathfrak{h}}$, and we use the same letters to denote these extensions. By an abuse of language, we say an element in $\widehat{\mathfrak{h}}$ is in $\operatorname{Ker}\widehat{\zeta}$ if each of its homogeneous components belongs to $\operatorname{Ker}\widehat{\zeta}$. Put $D := \sum_{m=1}^{\infty} \frac{D_m}{m}$ and $\overline{D} := \sum_{m=1}^{\infty} \frac{\overline{D}_m}{m}$. Both D and $\overline{D}$ are derivations of $\widehat{\mathfrak{h}}$. Furthermore, if we put $\sigma = \exp(D)$ and $\overline{\sigma} = \tau\sigma\tau = \exp(\overline{D})$, then σ and $\overline{\sigma}$ are automorphisms of $\widehat{\mathfrak{h}}$ (standard correspondence between derivation and homomorphism). Ohno's relation in this setting is stated as follows.

Theorem 5 (Ohno) *For any $w_0 \in \mathfrak{h}^0$, we have*

$$(\sigma - \overline{\sigma})(w_0) \in \operatorname{Ker}\widehat{\zeta}.$$

Proof. Since $D(x) = 0$ and $D(y) = (x + \frac{x^2}{2} + \frac{x^3}{3} + \cdots)y = (-\log(1-x))y$, we have $D^n(x) = 0, D^n(y) = (-\log(1-x))^n y$ and hence $\sigma(x) = x$ and $\sigma(y) = \sum_{n=0}^{\infty} \frac{1}{n!}(-\log(1-x))^n y = (1-x)^{-1}y = (1+x+x^2+x^3+\cdots)y$. From this, we have

$$\begin{aligned}
&\sigma(x^{k_1-1}yx^{k_2-1}y\cdots x^{k_n-1}y) \\
= \;& x^{k_1-1}(1+x+x^2+\cdots)yx^{k_2-1}(1+x+x^2+\cdots)y\cdots x^{k_n-1}(1+x+x^2+\cdots)y \\
= \;& \sum_{l=0}^{\infty} \sum_{\substack{e_1+e_2+\cdots+e_n=l \\ e_i\geq 0}} x^{k_1+e_1-1}yx^{k_2+e_2-1}y\cdots x^{k_n+e_n-1}y.
\end{aligned}$$

By Ohno [7], we conclude $(\sigma - \sigma\tau)(w_0) \in \operatorname{Ker}\widehat{\zeta}$ for any $w_0 \in \mathfrak{h}^0$. This in turn gives $(\sigma - \tau\sigma\tau)(w_0) \in \operatorname{Ker}\widehat{\zeta}$, since we have $(\sigma\tau - \tau\sigma\tau)(w_0) \in \operatorname{Ker}\widehat{\zeta}$ by duality. ∎

Remark Precisely speaking, Ohno's theorem [7, Theorem 1] is equivalent to Theorem 5 plus duality.

Proof of Theorem 4.

Put $\partial = \sum_{n=1}^{\infty} \frac{\partial_n}{n}$. This is a derivation of $\widehat{\mathfrak{h}}$. We prove the following formula.

Proposition 6 *We have*

$$\exp(\partial) = \overline{\sigma} \cdot \sigma^{-1}.$$

This relation shows that Theorem 4 is equivalent to Theorem 5, because from the identities $\partial = \log(\overline{\sigma}\cdot\sigma^{-1}) = \log(1-(\sigma-\overline{\sigma})\sigma^{-1})$ and $\sigma-\overline{\sigma} = (1-\overline{\sigma}\cdot\sigma^{-1})\sigma = (1-\exp(\partial))\sigma$ we have $\partial(\mathfrak{h}^0) = (\sigma - \overline{\sigma})(\mathfrak{h}^0)$.

Proof. One of our original proofs is essentially reproduced in [5] from a somewhat different viewpoint. Here we give another proof. We embed $\widehat{\mathfrak{h}}$ into $\widehat{\mathfrak{h}}_{\mathbf{R}} := \mathbf{R}\langle\langle x, y\rangle\rangle$. Put $z = x + y$. Consider a one parameter family ϕ^t ($t \in \mathbf{R}$) of automorphism of $\widehat{\mathfrak{h}}_{\mathbf{R}}$ defined by $\phi^t(z) = z$, $\phi^t(y) = (1-z)^t y(1 - \frac{1-(1-z)^t}{z} y)^{-1}$. We have $\phi^0 = 1$ and

(i) $\phi^s\phi^t = \phi^{s+t}$,

(ii) $\frac{d}{dt}\phi^t|_{t=0} = \partial$,

(iii) $\phi^1 = \overline{\sigma} \cdot \sigma^{-1}$.

For (i), put $\lambda = -\log(1-z)$. We only need to show $\phi^s\phi^t(y) = \phi^{s+t}(y)$:

$$\begin{aligned}
\phi^s(\phi^t(y)) &= \phi^s(e^{-\lambda t}y(1 - \frac{1-e^{-\lambda t}}{z}y)^{-1}) \\
&= e^{-\lambda t}\phi^s(y)(1 - \frac{1-e^{-\lambda t}}{z}\phi^s(y))^{-1} \\
&= e^{-\lambda t}e^{-\lambda s}y(1 - \frac{1-e^{-\lambda s}}{z}y)^{-1}(1 - \frac{1-e^{-\lambda t}}{z}e^{-\lambda s}y(1 - \frac{1-e^{-\lambda s}}{z}y)^{-1})^{-1} \\
&= e^{-\lambda(s+t)}y(1 - \frac{1-e^{-\lambda s}}{z}y - \frac{1-e^{-\lambda t}}{z}e^{-\lambda s}y)^{-1} \\
&= e^{-\lambda(s+t)}y(1 - \frac{1-e^{-\lambda(s+t)}}{z}y)^{-1} \\
&= \phi^{s+t}(y).
\end{aligned}$$

The left-hand side of (ii) is a derivation which sends z to 0. As for the image of y, the expansion

$$\begin{aligned}
\phi^t(y) &= (1 + \log(1-z)t + \cdots)y(1 + \frac{\log(1-z)}{z}yt + \cdots)^{-1} \\
&= y + (\log(1-z)y - y\frac{\log(1-z)}{z}y)t + O(t^2)
\end{aligned}$$

shows that

$$\frac{d}{dt}\phi^t|_{t=0}(y) = \log(1-z)y - y\frac{\log(1-z)}{z}y = x\frac{\log(1-z)}{z}y = -x\sum_{n=1}^{\infty}\frac{(x+y)^{n-1}}{n}y = \partial(y).$$

We saw in the proof of Theorem 5 that $\sigma(x) = x$ and $\sigma(y) = (1-x)^{-1}y$. From this we see that $\sigma^{-1}(x) = x$ and $\sigma^{-1}(y) = (1-x)y$. In a similar manner we get $\overline{\sigma}(x) = x(1-y)^{-1}$ and $\overline{\sigma}(y) = y$. Hence, $\overline{\sigma}\cdot\sigma^{-1}(x) = x(1-y)^{-1}$, $\overline{\sigma}\cdot\sigma^{-1}(y) = (1-x(1-y)^{-1})y = y - xy(1-y)^{-1}$ and $\overline{\sigma}\cdot\sigma^{-1}(z) = x(1-y)^{-1} + y - xy(1-y)^{-1} = z$. On the other hand, we have by definition $\phi^1(z) = z$ and $\phi^1(y) = (1-z)y(1-y)^{-1} = y - xy(1-y)^{-1}$. This proves (iii).

Now, a one parameter family satisfying (i) and (ii) is nothing but $\exp(t\partial)$, hence the proposition follows from (iii), and therefore completes the proof of Theorem 4 ∎

3 Regularized double shuffle relations

Two commutative multiplications which correspond to the product of MZVs are defined on the underlying vector space of $\mathfrak{h}$: one is the shuffle product ш coming from the shuffle product of iterated integrals (1), and the other is Hoffman's harmonic product $*$ ([4]) coming from the shuffle-like multiplication of series (2). We denote by $\mathfrak{h}_{sh}$ and $\mathfrak{h}_{har}$ the respective commutative algebras. Also, the subspaces $\mathfrak{h}^1$ and $\mathfrak{h}^0$ are closed under each of these multiplications and hence can be viewed as subalgebras which are denoted by $\mathfrak{h}^1_{sh}, \mathfrak{h}^0_{sh}, \mathfrak{h}^1_{har}$ and $\mathfrak{h}^0_{har}$. We know the structures of $\mathfrak{h}_{sh}$ and $\mathfrak{h}_{har}$ as commutative algebras (for $\mathfrak{h}_{sh}$ see, *e.g.*, [8, Theorem 6.1]), and [4] for $\mathfrak{h}_{har}$). In particular, we have the isomorphism

$$\mathfrak{h}_{sh} \simeq \mathfrak{h}^0_{sh}[x, y],$$

based on which is the following definition of the regularization. The right-hand side is viewed as the polynomial algebra over $\mathfrak{h}^0_{sh}$ generated by x and y (every product being the shuffle product).

Definition 7 *We define a* Q*-linear map* reg : $\mathfrak{h} \to \mathfrak{h}^0$, *the regularization map, by* reg(w) = *the constant term of the expression of* w *as an element of* $\mathfrak{h}^0_{sh}[x,y]$. *Clearly, when viewed as a map from* $\mathfrak{h}_{sh}$ *to* $\mathfrak{h}^0_{sh}$, *the* reg *is an algebra homomorphism:*

$$\mathrm{reg}(w_1 ш\, w_2) = \mathrm{reg}(w_1) ш\, \mathrm{reg}(w_2) \quad (w_1,\, w_2 \in \mathfrak{h}).$$

The reg *restricts to the identity map on* $\mathfrak{h}^0$.

We can describe more explicitly the images of words under reg as follows.

Proposition 8 (i) *For each word* $w \in \mathfrak{h}$, *write* $w = y^m w_0 x^n$ *with* $m, n \geq 0$ *and* $w_0 \in \mathfrak{h}^0$ *(*m, n, *and* w_0 *are uniquely determined by* w*). Then we have*

$$\mathrm{reg}(w) = \sum_{\substack{0\le i\le m\\ 0\le j\le n}} (-1)^{i+j} y^i ш\, y^{m-i} w_0 x^{n-j} ш\, x^j. \qquad (3)$$

(ii) *The formula* (3) *takes simpler form for special words*;

$$\begin{aligned}\mathrm{reg}(x^n) &= \mathrm{reg}(y^m)=0 \quad \textit{for } m,n\geq 1,\\ \mathrm{reg}(y^m x^n) &= (-1)^{m+n-1}x^n y^m \quad \textit{for } m,n\geq 1,\\ \mathrm{reg}(y^m w_0) &= (-1)^m x(y^m ш\, w_0') \quad \textit{for } m\geq 0,\ w_0=xw_0'\in\mathfrak{h}^0\\ \mathrm{reg}(w_0x^n) &= (-1)^n(w_0' ш\, x^n)y \quad \textit{for } n\geq 0,\ w_0=w_0'y\in\mathfrak{h}^0.\end{aligned}$$

(iii) *For a word* $w=y^m w_0 x^n$, $m,n\geq 0$, $w_0\in\mathfrak{h}^0$, *we have*

$$w=\sum_{\substack{0\leq i\leq m\\ 0\leq j\leq n}} \mathrm{reg}(y^{m-i}w_0x^{n-j})ш\, y^i ш\, x^j. \tag{4}$$

This gives the expression of w *as an element of* $\mathfrak{h}^0_{sh}[x,y]$.

Proof. For $w=y^m w_0 x^n$, denote the right-hand side of (3) by $\mathrm{reg}'(w)$. We show that $\mathrm{reg}'(w)\in\mathfrak{h}^0$ and the formula (4) for reg′;

$$w=\sum_{\substack{0\leq i\leq m\\ 0\leq j\leq n}} \mathrm{reg}'(y^{m-i}w_0x^{n-j})ш\, y^i ш\, x^j. \tag{5}$$

Then, by definition, we conclude that $\mathrm{reg}(w)=\mathrm{reg}'(w)$ and so (i) and (iii) is proved. In the course of calculation, (ii) is also proved.

Put $v_i=\sum_{j=0}^n(-1)^j y^{m-i}w_0x^{n-j}ш\, x^j$ so that $\mathrm{reg}'(w)=\sum_{i=0}^m(-1)^i y^i ш\, v_i$. We first compute v_i by using the inductive structure of the shuffle product. The case $w_0=1$ ($w=y^mx^n$) will be treated separately, so put $w_0=xw_0'y$.

$$\begin{aligned} v_i &= y^{m-i}w_0x^n+\sum_{j=1}^{n-1}(-1)^j y^{m-i}w_0x^{n-j}ш\, x^j+(-1)^n y^{m-i}w_0ш\, x^n\\ &= y^{m-i}w_0x^n+\sum_{j=1}^{n-1}(-1)^j((y^{m-i}w_0x^{n-j}ш\, x^{j-1})x+(y^{m-i}w_0x^{n-j-1}ш\, x^j)x)\\ &\quad +(-1)^n((y^{m-i}w_0ш\, x^{n-1})x+(y^{m-i}xw_0'ш\, x^n)y)\\ &= \sum_{j=1}^{n}(-1)^j(y^{m-i}w_0x^{n-j}ш\, x^{j-1})x+\sum_{j=0}^{n-1}(-1)^j(y^{m-i}w_0x^{n-j-1}ш\, x^j)x\\ &\quad +(-1)^n(y^{m-i}xw_0'ш\, x^n)y\\ &= (-1)^n(y^{m-i}xw_0'ш\, x^n)y.\end{aligned}$$

Thus, $v_i\in\mathfrak{h}^1$ and so $\mathrm{reg}'(w)=\sum_{i=0}^m(-1)^i y^i ш\, v_i\in\mathfrak{h}^1$. The above computation also proves (after we conclude reg = reg′) the formula for $\mathrm{reg}(w_0x^n)$ in (ii) (set $m=0$ and $xw_0\to w_0$). By a similar calculation of $\sum_{i=0}^m(-1)^i y^i ш\, y^{m-i}w_0x^{n-j}$, we can show that $\mathrm{reg}'(w)\in x\mathfrak{h}$ as well as the formula for $\mathrm{reg}(y^mw_0)$. We therefore conclude $\mathrm{reg}'(w)\in\mathfrak{h}^0$.

Now we prove the formula (5). By definition,

$$\mathrm{reg}'(y^{m-i}w_0x^{n-j})=\sum_{\substack{0\leq k\leq m-i\\ 0\leq l\leq n-j}}(-1)^{k+l}y^kш\, y^{m-i-k}w_0x^{n-j-l}ш\, x^l.$$

Putting $i+k=s, j+l=t$, we have

$$\begin{aligned}
&\sum_{\substack{0\le i\le m\\0\le j\le n}} \mathrm{reg}'(y^{m-i}w_0x^{n-j}) ш\, y^i ш\, x^j \\
&= \sum_{\substack{0\le i\le m\\0\le j\le n}} \left(\sum_{\substack{0\le k\le m-i\\0\le l\le n-j}} (-1)^{k+l} y^k ш\, y^{m-i-k} w_0 x^{n-j-l} ш\, x^l \right) ш\, y^i ш\, x^j \\
&= \sum_{\substack{0\le s\le m\\0\le t\le n}} \sum_{\substack{0\le k\le s\\0\le l\le t}} (-1)^{k+l} y^k ш\, y^{m-s} w_0 x^{n-t} ш\, x^l ш\, y^{s-k} ш\, x^{t-l} \\
&= \sum_{\substack{0\le s\le m\\0\le t\le n}} \sum_{\substack{0\le k\le s\\0\le l\le t}} (-1)^{k+l} \binom{s}{k} y^s ш \binom{t}{l} x^t ш\, y^{m-s} w_0 x^{n-t} \\
&= \sum_{\substack{0\le s\le m\\0\le t\le n}} \left(\sum_{k=0}^{s} (-1)^k \binom{s}{k} y^s \right) ш \left(\sum_{l=0}^{t} (-1)^l \binom{t}{l} x^t \right) ш\, y^{m-s} w_0 x^{n-t}.
\end{aligned}$$

Since $\left(\sum_{k=0}^{s}(-1)^k\binom{s}{k}y^s\right) ш \left(\sum_{l=0}^{t}(-1)^l\binom{t}{l}x^t\right) = 0$ if $s>0$ or $t>0$, and $=1$ if $s=t=0$, we have

$$\sum_{\substack{0\le i\le m\\0\le j\le n}} \mathrm{reg}'(y^{m-i}w_0x^{n-j}) ш\, y^i ш\, x^j = y^m w_0 x^n = w.$$

Thus we have established $\mathrm{reg} = \mathrm{reg}'$.

If $w = x^n$, we see by definition that $\mathrm{reg}(x^n) = \mathrm{reg}'(x^n) = \sum_{j=0}^{n}(-1)^j x^{n-j} ш\, x^j = \sum_{j=0}^{n}(-1)^j\binom{n}{j}x^n = 0$. Similarly we have $\mathrm{reg}(y^m) = \mathrm{reg}'(y^m) = 0$. For $\mathrm{reg}(y^m x^n)$, we first calculate $\sum_{i=0}^{m}(-1)^i y^i ш\, y^{m-i}x^{n-j}$. If $j=n$, then $\sum_{i=0}^{m}(-1)^i y^i ш\, y^{m-i} = \sum_{i=0}^{m}(-1)^i\binom{m}{i}y^m = 0$. For $j<n$,

$$\begin{aligned}
&\sum_{i=0}^{m}(-1)^i y^i ш\, y^{m-i}x^{n-j} \\
&= y^m x^{n-j} + \sum_{i=1}^{m-1}(-1)^i y^i ш\, y^{m-i}x^{n-j} + (-1)^m y^m ш\, x^{n-j} \\
&= y^m x^{n-j} + \sum_{i=1}^{m-1}(-1)^i (y(y^{i-1} ш\, y^{m-i}x^{n-j}) + y(y^i ш\, y^{m-i-1}x^{n-j})) \\
&\quad +(-1)^m (y(y^{m-1} ш\, x^{n-j}) + x(y^m ш\, x^{n-j-1})) \\
&= \sum_{i=1}^{m}(-1)^i y(y^{i-1} ш\, y^{m-i}x^{n-j}) + \sum_{i=0}^{m-1}(-1)^i y(y^i ш\, y^{m-i-1}x^{n-j}) + (-1)^m x(y^m ш\, x^{n-j-1}) \\
&= (-1)^m x(y^m ш\, x^{n-j-1}).
\end{aligned}$$

Hence,

$$\begin{aligned}
\mathrm{reg}(y^m x^n) &= \sum_{j=0}^{n}(-1)^j x^j ш \left(\sum_{i=0}^{m}(-1)^i y^i ш\, y^{m-i}x^{n-j}\right) \\
&= \sum_{j=0}^{n-1}(-1)^j x^j ш \left((-1)^m x(y^m ш\, x^{n-j-1})\right) \\
&= (-1)^m \sum_{j=0}^{n-1}(-1)^j x^j ш\, x(y^m ш\, x^{n-j-1}).
\end{aligned}$$

If $n = 1$, this is equal to $(-1)^m xy^m$. Assume $n \geq 2$. We further compute the last sum by expanding the shuffle products;

$$\begin{aligned}
&\sum_{j=0}^{n-1}(-1)^j x^j ш\, x(y^m ш\, x^{n-j-1}) \\
&= x(y^m ш\, x^{n-1}) + \sum_{j=1}^{n-1}(-1)^j \left(x(x^{j-1} ш\, x(y^m ш\, x^{n-j-1})) + x(x^j ш\, y^m ш\, x^{n-j-1})\right) \\
&= \sum_{j=1}^{n-1}(-1)^j x(x^{j-1} ш\, x(y^m ш\, x^{n-j-1})) + x\sum_{j=0}^{n-1}(-1)^j y^m ш\, x^j ш\, x^{n-j-1} \\
&= \sum_{j=1}^{n-1}(-1)^j x(x^{j-1} ш\, x(y^m ш\, x^{n-j-1})) \quad \left(\sum_{j=0}^{n-1}(-1)^j y^m ш\, x^j ш\, x^{n-j-1} = y^m ш \sum_{j=0}^{n-1}(-1)^j \tbinom{n-1}{j} x^{n-1} = 0\right) \\
&= -x\sum_{j=0}^{n-2}(-1)^j x^j ш\, x(y^m ш\, x^{n-j-2}).
\end{aligned}$$

Repeating this, we have

$$\begin{aligned}
\sum_{j=0}^{n-1}(-1)^j x^j ш\, x(y^m ш\, x^{n-j-1}) &= -x\sum_{j=0}^{n-2}(-1)^j x^j ш\, x(y^m ш\, x^{n-j-2}) \\
&= (-1)^2 x^2 \sum_{j=0}^{n-3}(-1)^j x^j ш\, x(y^m ш\, x^{n-j-3}) \\
&= \cdots \\
&= (-1)^{n-1} x^n y^m.
\end{aligned}$$

Thus we have proved $\mathrm{reg}(y^m x^n) = (-1)^{m+n-1} x^n y^m$. ∎

We now state the regularized double shuffle relations.

Theorem 9 *For any $w \in \mathfrak{h}^1$ and any $w_0 \in \mathfrak{h}^0$, we have*

$$\mathrm{reg}(w * w_0 - w ш\, w_0) \in \mathrm{Ker}\,\widehat{\zeta}.$$

When $w \in \mathfrak{h}^0$, this reduces to the usual double shuffle relations

$$w * w_0 - w ш\, w_0 \in \mathrm{Ker}\,\widehat{\zeta}.$$

Conjecture *Regularized double shuffle relations supply all linear relations of MZVs:*

$$\langle \mathrm{reg}(w * w_0 - w ⧢ w_0) \mid w \in \mathfrak{h}^1,\, w_0 \in \mathfrak{h}^0 \rangle_{\mathbf{Q}} = \mathrm{Ker}\,\widehat{\zeta}.$$

Remark We checked by computer that these relations are enough to reduce the dimension of MZVs to the conjectural value ([9]) up to weight 12.

For the proof of the theorem we introduce certain extensions of $\widehat{\zeta}$ to both $\mathfrak{h}^1_{sh}$ and $\mathfrak{h}^1_{har}$.

Proposition 10 *There exist* $\mathbf{Q}$*-algebra homomorphisms into the polynomial algebra* $\mathbf{R}[\mathrm{T}]$

$$\begin{aligned} \widehat{Z}_{sh} &: \mathfrak{h}^1_{sh} \longrightarrow \mathbf{R}[\mathrm{T}] \\ \widehat{Z}_{har} &: \mathfrak{h}^1_{har} \longrightarrow \mathbf{R}[\mathrm{T}] \end{aligned}$$

which are uniquely characterized by the properties that they extend $\widehat{\zeta} : \mathfrak{h}^0 \to \mathbf{R}$ *(i.e.* $\widehat{Z}_{sh}(w_0) = \widehat{Z}_{har}(w_0) = \widehat{\zeta}(w_0)$ *for* $w_0 \in \mathfrak{h}^0$*) and that* $\widehat{Z}_{sh}(y) = T$, $\widehat{Z}_{har}(y) = T$.

Proof. This is clear from the isomorphisms $\mathfrak{h}^1_{sh} \simeq \mathfrak{h}^0_{sh}[y]$ and $\mathfrak{h}^1_{har} \simeq \mathfrak{h}^0_{har}[y]$ ([8] and [4]) and the fact that the $\widehat{\zeta}$ is an algebra homomorphism for both shuffle and harmonic products. ∎

The key to prove Theorem 9 is the following theorem due to Zagier.

Theorem 11 (Zagier) *There exists an* $\mathbf{R}$*-linear map* $\rho : \mathbf{R}[\mathrm{T}] \to \mathbf{R}[\mathrm{T}]$ *such that*

$$\widehat{Z}_{sh} = \rho \circ \widehat{Z}_{har}.$$

Specifically, each $\rho(T^l)$ *is given by the generating series*

$$\sum_{l=0}^{\infty} \rho(T^l) \frac{u^l}{l!} = \exp(Tu) \cdot \exp\Big(\sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} u^n\Big).$$

Thus the coefficients of the polynomial $\rho(T^l) = T^l + O(T^{l-2})$ *for each* l *belong to the* $\mathbf{Q}$*-algebra generated by Riemann zeta values, and the coefficient of* T^{l-k} *is of weight* k*.*

Proof. We reproduce here Zagier's proof with his permission. The idea is to compare the asymptotic behaviors of

$$\sum_{\substack{M > m_1 > m_2 > \cdots > m_n > 0 \\ m_i \in \mathbf{Z}}} \frac{1}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}} \quad \text{as } M \to \infty$$

and

$$\int \cdots \int_{x > t_1 > t_2 > \cdots > t_k > 0} \frac{dt_1}{A_1(t_1)} \frac{dt_2}{A_2(t_2)} \cdots \frac{dt_k}{A_k(t_k)} \quad \text{as } x \to 1,$$

where $k = k_1 + k_2 + \cdots + k_n$ and $A_i(t) = 1 - t$ if $i \in \{k_1, k_1 + k_2, \ldots, k_1 + k_2 + \cdots + k_n\}$ and $A_i(t) = t$ otherwise.

For that purpose, put

$$\zeta_M(k_1, k_2, \ldots, k_n) := \sum_{M > m_1 > m_2 > \cdots > m_n > 0} \frac{1}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}}$$

for $M > 0$ and an index set $\mathrm{k} = (k_1, k_2, \ldots, k_n)$ (we allow $k_1 = 1$). If k is admissible, i.e., $k_1 > 1$, $\zeta_M(\mathrm{k})$ converges to $\zeta(\mathrm{k})$ as $M \to \infty$. We note that we can write the product $\zeta_M(\mathrm{k})\zeta_M(\mathrm{k}')$ as a linear combination of $\zeta_M(\mathrm{k}'')$'s by the same rule (based on which the harmonic product on $\mathfrak{h}$ is defined) as in the case of original infinite series of multiple zeta values. For instance, we have

$$\zeta_M(k)\zeta_M(k') = \zeta_M(k, k') + \zeta_M(k', k) + \zeta_M(k + k').$$

With this fact and the classical formula

$$\zeta_M(1) = 1 + \frac{1}{2} + \cdots + \frac{1}{M-1} = \log M + \gamma + O(\frac{1}{M}) \quad (\gamma = \text{ Euler's constant}), \tag{6}$$

we see inductively that for any index set $\mathbf{k}$ there uniquely exists a polynomial $\alpha_{\mathrm{k}}(T) \in \mathbf{R}[\mathrm{T}]$ such that

$$\lim_{M \to \infty} M^{\delta} \left(\zeta_M(\mathrm{k}) - \alpha_{\mathrm{k}}(\log M + \gamma) \right) = 0 \tag{7}$$

for some $\delta > 0$ (δ depends on k). Under the correspondence $\mathbf{k} = (k_1, k_2, \ldots, k_n) \leftrightarrow w = x^{k_1 - 1} y x^{k_2 - 1} y \cdots x^{k_n - 1} y$ of index sets and words in $\mathfrak{h}^1$, this $\alpha_{\mathrm{k}}(T)$ is nothing but $\widehat{Z}_{har}(w)$. Furthermore, we can show by induction on the number of first consecutive 1's in the index set that, for $\mathrm{k} = (\underbrace{1, 1, \ldots, 1}_{s}, \mathrm{k}')$ with k' admissible,

$$\alpha_{\mathrm{k}}(T) = \zeta(\mathrm{k}') \frac{T^s}{s!} + (\text{terms of lower degree})$$

and that the coefficient of T^i in $\alpha_{\mathrm{k}}(T)$ is a $\mathbf{Q}$-linear combination of multiple zeta values of weight $k - i$ ($k =$ weight of k).

Example By (6), $\alpha_1(T) = T$. From this and $\zeta_M(1)\zeta_M(1) = 2\zeta_M(1,1) + \zeta_M(2)$, we obtain $\alpha_{1,1}(T) = T^2/2 - \zeta(2)/2$.

Next, for $\mathrm{k} = (k_1, k_2, \ldots, k_n)$ and $0 < x < 1$, put

$$Li_{\mathrm{k}}(x) = \int \cdots \int_{x > t_1 > t_2 > \cdots > t_k > 0} \frac{dt_1}{A_1(t_1)} \frac{dt_2}{A_2(t_2)} \cdots \frac{dt_k}{A_k(t_k)},$$

where $A_i(t)$ are determined as above. Step-by-step integration shows that

$$Li_{\mathrm{k}}(x) = \sum_{m_1 > m_2 > \cdots > m_n > 0} \frac{x^{m_1}}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}}.$$

The product $Li_{\mathbf{k}}(x)Li_{\mathbf{k}'}(x)$ is a linear combination of $Li_{\mathbf{k}''}(x)$'s via the shuffle product identity. Starting with $Li_1(x) = -\log(1-x)$, similar inductive argument shows that, for each index set k, there uniquely exists a polynomial $\beta_{\mathbf{k}}(T) \in \mathbf{R}[\mathrm{T}]$ such that

$$\lim_{x\to 1}(1-x)^{-\delta}\left(Li_{\mathbf{k}}(x) - \beta_{\mathbf{k}}\left(-\log(1-x)\right)\right) = 0$$

for some $\delta > 0$, and that $\beta_{\mathbf{k}}(T) = \widehat{Z}_{sh}(w)$ if k corresponds to w.

Example Since $Li_{\underbrace{1,\ldots,1}_{s}}(x) = Li_1(x)^s/s!$, $\beta_{\underbrace{1,\ldots,1}_{s}}(T) = T^s/s!$. By $Li_2(x)Li_1(x) = Li_{1,2}(x) + 2Li_{2,1}(x)$, we have $\beta_{1,2}(T) = \zeta(2)T - 2\zeta(2,1)$.

We now prove Theorem 11, which asserts the existence of an R-linear map $\rho : \mathbf{R}[\mathrm{T}] \to \mathbf{R}[\mathrm{T}]$ such that $\beta_{\mathbf{k}}(T) = \rho(\alpha_{\mathbf{k}}(T))$. First,

$$\begin{aligned} Li_{\mathbf{k}}(x) &= \sum_{m_1>m_2>\cdots>m_n>0} \frac{x^{m_1}}{m_1^{k_1}m_2^{k_2}\cdots m_n^{k_n}} \\ &= \sum_{m=1}^{\infty}\left(\sum_{m>m_2>\cdots>m_n>0}\frac{1}{m^{k_1}m_2^{k_2}\cdots m_{n-1}^{k_{n-1}}m_n{}^{k_n}}\right)x^m \\ &= \sum_{m=1}^{\infty}\left(\zeta_{m+1}(\mathbf{k}) - \zeta_m(\mathbf{k})\right)x^m \\ &= \sum_{m=1}^{\infty}\zeta_m(\mathbf{k})(x^{m-1} - x^m) \\ &= (x^{-1}-1)\sum_{m=1}^{\infty}\zeta_m(\mathbf{k})x^m, \end{aligned}$$

empty sum as $\zeta_1(\mathbf{k})$ being regarded as 0. Putting $x = e^{-\varepsilon}$, we have

$$Li_{\mathbf{k}}(e^{-\varepsilon}) = (e^{\varepsilon}-1)\sum_{m=1}^{\infty}\zeta_m(\mathbf{k})e^{-\varepsilon m}.$$

By (7), there exist positive constants c and δ such that

$$|\zeta_m(\mathbf{k}) - \alpha_{\mathbf{k}}(\log m + \gamma)| \le cm^{-\delta}$$

for all $m \ge 1$. Since the function $x^{-\delta}e^{-\varepsilon x}$ for $x > 0$ is positive and monotone decreasing, we have

$$0 < \sum_{m=1}^{\infty} m^{-\delta}e^{-\varepsilon m} < \int_0^{\infty} x^{-\delta}e^{-\varepsilon x}dx = \varepsilon^{\delta-1}\Gamma(1-\delta).$$

From this and $e^{\varepsilon} - 1 = \varepsilon + O(\varepsilon^2)$, we obtain

$$\lim_{\varepsilon\to 0}\varepsilon^{-\delta/2}(e^{\varepsilon}-1)\sum_{m=1}^{\infty}m^{-\delta}e^{-\varepsilon m} = 0.$$

Thus

$$\lim_{\varepsilon\to 0}\varepsilon^{-\delta/2}\left((e^{\varepsilon}-1)\sum_{m=1}^{\infty}\zeta_m(\mathrm{k})e^{-\varepsilon m}-(e^{\varepsilon}-1)\sum_{m=1}^{\infty}\alpha_{\mathrm{k}}(\log m+\gamma)e^{-\varepsilon m}\right)=0$$

or

$$\lim_{\varepsilon\to 0}\varepsilon^{-\delta/2}\left(Li_{\mathrm{k}}(e^{-\varepsilon})-(e^{\varepsilon}-1)\sum_{m=1}^{\infty}\alpha_{\mathrm{k}}(\log m+\gamma)e^{-\varepsilon m}\right)=0.$$

Since $1-x=\varepsilon+O(\varepsilon^2)$ and $-\log(1-x)=-\log\varepsilon+O(\varepsilon)$ $(\varepsilon\to 0,\ x=e^{-\varepsilon})$, the last equality and the definition of $\beta_{\mathrm{k}}(T)$ implies

$$\lim_{\varepsilon\to 0}\left(\beta_{\mathrm{k}}(-\log\varepsilon)-(e^{\varepsilon}-1)\sum_{m=1}^{\infty}\alpha_{\mathrm{k}}(\log m+\gamma)e^{-\varepsilon m}\right)=0. \tag{8}$$

Lemma 12 *For any integer $l\geq 0$, we have*

$$\sum_{m=1}^{\infty}(\log m)^l e^{-\varepsilon m}=\frac{1}{\varepsilon}\sum_{j=0}^{l}\binom{l}{j}\Gamma^{(j)}(1)(-\log\varepsilon)^{l-j}+O(1)\quad \textit{as } \varepsilon\to 0.$$

Proof. By the Euler-Maclaurin formula,

$$\sum_{m=1}^{\infty}(\log m)^l e^{-\varepsilon m}=\int_0^{\infty}(\log x)^l e^{-\varepsilon x}dx+O(1),\quad \text{as } \varepsilon\to 0.$$

Changing the variable x to x/ε, we obtain

$$\begin{aligned}\int_0^{\infty}(\log x)^l e^{-\varepsilon x}dx&=\frac{1}{\varepsilon}\int_0^{\infty}(\log x-\log\varepsilon)^l e^{-x}dx\\&=\frac{1}{\varepsilon}\sum_{j=0}^{l}\binom{l}{j}(-\log\varepsilon)^{l-j}\int_0^{\infty}(\log x)^j e^{-x}dx.\end{aligned}$$

Since

$$\begin{aligned}\int_0^{\infty}(\log x)^j e^{-x}dx&=\int_0^{\infty}\left(\left(\frac{d}{ds}\right)^j x^{s-1}\right)\Bigg|_{s=1}e^{-x}dx\\&=\left(\left(\frac{d}{ds}\right)^j\Gamma(s)\right)\Bigg|_{s=1}\\&=\Gamma^{(j)}(1),\end{aligned}$$

we proved Lemma. ∎

Now put $P_l(T) := \sum_{j=0}^{l} \binom{l}{j} \Gamma^{(j)}(1) T^{l-j}$. Then, by the lemma and $e^\varepsilon - 1 = \varepsilon + O(\varepsilon^2)$, we have

$$\lim_{\varepsilon \to 0} \left((e^\varepsilon - 1) \sum_{m=1}^{\infty} (\log m)^l e^{-\varepsilon m} - P_l(-\log \varepsilon) \right) = 0. \tag{9}$$

If we write $\alpha_{\mathbf{k}}(T) = \sum_{l=0}^{s} a_l (T-\gamma)^l$, then $\alpha_{\mathbf{k}}(\log m + \gamma) = \sum_{l=0}^{s} a_l (\log m)^l$ and from (8) and (9) we obtain

$$\lim_{\varepsilon \to 0} \left(\beta_{\mathbf{k}}(-\log \varepsilon) - \sum_{l=0}^{s} a_l P_l(-\log \varepsilon) \right) = 0.$$

Therefore, the polynomial $\beta_{\mathbf{k}}(T)$ is obtained from $\alpha_{\mathbf{k}}(T)$ by writing it as a polynomial in $T-\gamma$ and replacing $(T-\gamma)^l$ by $P_l(T)$. Since $T^l = (T-\gamma+\gamma)^l = \sum_{j=0}^{l} \binom{l}{j} \gamma^{l-j} (T-\gamma)^j$, this amounts to replacing T^l by $\sum_{j=0}^{l} \binom{l}{j} \gamma^{l-j} P_j(T)$. Thus we have shown that if we define the $\mathbf{R}$-linear map ρ by $\rho(T^l) = \sum_{j=0}^{l} \binom{l}{j} \gamma^{l-j} P_j(T)$, we get $\beta_{\mathbf{k}}(T) = \rho(\alpha_{\mathbf{k}}(T))$.

A generating function of $\rho(T^l)$ is given as follows.

$$\begin{aligned}
\sum_{l=0}^{\infty} \rho(T^l) \frac{u^l}{l!} &= \sum_{l=0}^{\infty} \sum_{j=0}^{l} \binom{l}{j} \gamma^{l-j} P_j(T) \frac{u^l}{l!} \\
&= \sum_{l=0}^{\infty} \sum_{j=0}^{l} \frac{(\gamma u)^{l-j}}{(l-j)!} \frac{P_j(T)}{j!} u^j \\
&= e^{\gamma u} \sum_{m=0}^{\infty} P_m(T) \frac{u^m}{m!} \\
&= e^{\gamma u} \sum_{m=0}^{\infty} \sum_{j=0}^{m} \binom{m}{j} \Gamma^{(j)}(1) T^{m-j} \frac{u^m}{m!} \\
&= e^{\gamma u} \sum_{m=0}^{\infty} \sum_{j=0}^{m} \frac{(Tu)^{m-j}}{(m-j)!} \Gamma^{(j)}(1) \frac{u^j}{j!} \\
&= e^{\gamma u} e^{Tu} \Gamma(1+u).
\end{aligned}$$

The classical formula $\Gamma(1+u) = \exp(-\gamma u + \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} u^n)$ yields

$$\sum_{l=0}^{\infty} \rho(T^l) \frac{u^l}{l!} = e^{Tu} \exp(\sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} u^n).$$

This completes the proof of the theorem. ∎

Example $\rho(T) = T$, $\rho(T^2) = T^2 + \zeta(2)$, $\rho(T^3) = T^3 + 3\zeta(2)T - 2\zeta(3)$, $\rho(T^4) = T^4 - 6\zeta(2)T^2 - 8\zeta(3)T + 6\zeta(4) + 3\zeta(2)^2$.

Remark The inverse ρ^* of ρ is given by

$$\sum_{l=0}^{\infty} \rho^*(T^l)\frac{u^l}{l!} = \exp(Tu)\exp\left(-\sum_{n=2}^{\infty}(-1)^n\frac{\zeta(n)}{n}u^n\right).$$

$\alpha_{\mathbf{k}}(T)$ is obtained from $\beta_{\mathbf{k}}(T)$ by $T^l \to \rho^*(T^l)$.

Proof of Theorem 9. For $w \in \mathfrak{h}^1$ and $w_0 \in \mathfrak{h}^0$, we prove a stronger statement that

$$\widehat{Z}_{sh}(w * w_0 - w ш w_0) = 0. \tag{10}$$

The constant term of $\widehat{Z}_{sh}(w)$ is $\widehat{\zeta}(\mathrm{reg}(w))$ and hence the theorem follows from this.

By Zagier's theorem, we have

$$\widehat{Z}_{sh}(w) - \rho(\widehat{Z}_{har}(w)) = 0$$

. Multiplying $\widehat{\zeta}(w_0)(= \widehat{Z}_{sh}(w_0) = \widehat{Z}_{har}(w_0)$, using the $\mathbf{R}$-linearity of ρ and the fact that both $\widehat{Z}_{sh}$ and $\widehat{Z}_{har}$ are algebra homomorphisms with respect to ш and $*$ respectively, we obtain

$$\widehat{Z}_{sh}(w_0 ш w) - \rho(\widehat{Z}_{har}(w_0 * w)) = 0.$$

Using again Zagier's theorem that $\rho(\widehat{Z}_{har}(w_0 * w)) = \widehat{Z}_{sh}(w_0 * w)$, we have proved (10). ∎

On $\mathfrak{h}^1$, we can consider a "harmonic regularization" based on the isomorphism $\mathfrak{h}^1_{har} \simeq \mathfrak{h}^0_{har}[y]$. Let $\mathrm{reg}_{har} : \mathfrak{h}^1 \to \mathfrak{h}^0$ be the $\mathbf{Q}$-linear map defined by $\mathrm{reg}_{har}(w) =$ the constant term of w expressed as an element of $\mathfrak{h}^0_{har}[y]$. The map reg_{har} is an algebra homomorphism with respect to the harmonic product $*$:

$$\mathrm{reg}_{har}(w_1 * w_2) = \mathrm{reg}_{har}(w_1) * \mathrm{reg}_{har}(w_2) \quad (w_1, w_2 \in \mathfrak{h}^1).$$

Proposition 13 *For $w = y^m w_0$ with $m \geq 0, w_0 \in \mathfrak{h}^0$, we have*

$$\mathrm{reg}_{har}(y^m w_0) = \sum_{i=0}^{m}(-1)^i\frac{y^{*i}}{i!} * y^{m-i}w_0$$

and

$$w = \sum_{0\leq i\leq m} \mathrm{reg}_{har}(y^{m-i}w_0) * \frac{y^{*i}}{i!},$$

where $y^{*i} = \underbrace{y * y * \cdots * y}_{i}.$

Proof. Omitted.

Let ϕ_i be homogeneous of degree i with

$$\exp_{har}\left(\sum_{r=1}^{\infty}(-1)^r\frac{x^{r-1}y}{r}\right) = \sum_{i=0}^{\infty}\phi_i,$$

where $\exp_{har}$ is an exponential in $\widehat{\mathfrak{h}}_{har}$, the completion of $\mathfrak{h}_{har}$. Zagier's theorem is then formulated as

$$\widehat{Z}_{sh}(w) = \widehat{Z}_{har}\Big(\sum_{0\le i\le m} \mathrm{reg}_{har}(y^{m-i}w_0) * \phi_i\Big) \quad (w = y^m w_0 \in \mathfrak{h}^1,\ m \ge 0,\ w_0 \in \mathfrak{h}^0).$$

4 Alternative Description of Regularization

The regularization map defined in the previous section can be described, at least on $\mathfrak{h}^1$, in terms of certain derivations.

Definition 14 *Define four derivations δ_s, $\overline{\delta_s}$, δ_h, $\overline{\delta_h} \in \mathrm{Der}(\mathfrak{h})$ by*

$$\delta_s : \begin{array}{l} x \longmapsto -xy \\ y \longmapsto -y^2, \end{array} \qquad \delta_h : \begin{array}{l} x \longmapsto 0 \\ y \longmapsto -xy - y^2, \end{array}$$

and $\overline{\delta_s} = \tau\delta_s\tau$, $\overline{\delta_h} = \tau\delta_h\tau$, where τ is the involution on $\mathfrak{h}$ defined in §2.

Theorem 15 (i) *For $w = y^m w_0$ with $m \ge 0$, $w_0 \in \mathfrak{h}^0$, we have*

$$\mathrm{reg}(w) = \frac{1}{m!}\delta_s^m(w_0).$$

(ii) *For $w = w_0 x^n$ with $n \ge 0$, $w_0 \in \mathfrak{h}^0$, we have*

$$\mathrm{reg}(w) = \frac{1}{n!}\overline{\delta_s}^n(w_0).$$

Remark Put $z_i = x^{i-1}y$ for $i \ge 1$. It is easily computed that $\overline{\delta_s}(z_i) = -iz_{i+1}$ (and $\delta_s(z_i) = -z_i z_1 - \sum_{j=2}^{i} z_j z_{i+1-j}$, $\delta_h(z_i) = -z_{i+1} - z_i z_1$, $\overline{\delta_h}(z_i) = -(i-1)z_{i+1} - \sum_{j=2}^{i} z_j z_{i+1-j}$). Thus the formula in (ii) is nothing but a description of the regularization given in [1] and (i) is its "dual".

Proposition 16 *For any $w \in \mathfrak{h}$, we have*

$$\delta_s(w) = yw - y ш w \quad \textit{and} \quad \delta_h(w) = yw - y * w.$$

Proof. By the definition of the shuffle product ш, it is clear that

$$y ш (w_1 w_2) = (y ш w_1)w_2 + w_1(y ш w_2) - w_1 y w_2$$

for any $w_1, w_2 \in \mathfrak{h}$. From this we see that the map $w \mapsto yw - y ш w$ defines a derivation on $\mathfrak{h}$ and hence is equal to δ_s because the images of x and y coincide.

As for δ_h, we can show the analogous identity

$$y * (w_1 w_2) = (y * w_1)w_2 + w_1(y * w_2) - w_1 y w_2$$

for any $w_1, w_2 \in \mathfrak{h}$ and the same arguments lead to the conclusion. ∎

Lemma 17 *For $m, n \geq 1$, we have*

$$\frac{1}{m!}\delta_s^m(w_0) = (-1)^m(y^m \mathbin{\sqcup\!\sqcup} w_0 - y(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0))$$

and

$$\frac{1}{n!}\overline{\delta_s}^n(w_0) = (-1)^n(w_0 \mathbin{\sqcup\!\sqcup} x^n - (w_0 \mathbin{\sqcup\!\sqcup} x^{n-1})x).$$

Proof. We prove the first identity by induction on m. The proof is completely similar for the other one. The case $m = 1$ is the above proposition. Assuming the equality for m, we compute by using Proposition 16

$$\begin{aligned}
&\frac{1}{m!}\delta_s^{m+1}(w_0) = \delta_s\left((-1)^m\left(y^m \mathbin{\sqcup\!\sqcup} w_0 - y(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0)\right)\right)\\
= \ & (-1)^m\left\{y\left(y^m \mathbin{\sqcup\!\sqcup} w_0 - y(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0)\right) - y \mathbin{\sqcup\!\sqcup} \left(y^m \mathbin{\sqcup\!\sqcup} w_0 - y(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0)\right)\right\}\\
= \ & (-1)^m\left\{y(y^m \mathbin{\sqcup\!\sqcup} w_0) - y^2(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0) - (m+1)y^{m+1} \mathbin{\sqcup\!\sqcup} w_0 + y^2(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0) + y(y \mathbin{\sqcup\!\sqcup} y^{m-1} \mathbin{\sqcup\!\sqcup} w_0)\right)\right\}\\
= \ & (-1)^m\left\{(m+1)y(y^m \mathbin{\sqcup\!\sqcup} w_0) - (m+1)y^{m+1} \mathbin{\sqcup\!\sqcup} w_0\right\}\\
= \ & (-1)^{m+1}(m+1)\left(y^{m+1} \mathbin{\sqcup\!\sqcup} w_0 - y(y^m \mathbin{\sqcup\!\sqcup} w_0)\right).
\end{aligned}$$

Hence we have

$$\frac{1}{(m+1)!}\delta_s^{m+1}(w_0) = (-1)^{m+1}\left(y^{m+1} \mathbin{\sqcup\!\sqcup} w_0 - y(y^m \mathbin{\sqcup\!\sqcup} w_0)\right)$$

and the lemma is proved. ∎

Proof of Theorem. By linearity, it suffices to prove the theorem for a word w_0. If $w_0 = 1$, the theorem is obvious since $\mathrm{reg}(y^m) = 0$ for $m \geq 1$ from Proposition 8 (ii). Put $w_0 = xw_0'$, $w_0' \in \mathfrak{h}^1$. Then, since $y^m \mathbin{\sqcup\!\sqcup} w_0 - y(y^{m-1} \mathbin{\sqcup\!\sqcup} w_0) = x(y^m \mathbin{\sqcup\!\sqcup} w_0')$, (i) follows from the lemma and Proposition 8 (ii). Proof of (ii) is omitted since it is proved similarly. ∎

Experiments in small degrees suggests that the derivation ∂_n introduced in §2 may be written in terms of newly introduced derivations. We propose the following conjecture.

Conjecture *The derivation ∂_n is contained for all $n \geq 1$ in the Lie subalgebra of* $\mathrm{Der}(\mathfrak{h})$ *generated by $\delta_s, \delta_h, \overline{\delta_s}$ and $\overline{\delta_h}$.*

Here are some relations among the derivations.

Proposition 18 (i) $\delta_s + \overline{\delta_s} = \delta_h + \overline{\delta_h}$.

(ii) $\partial_1 = \delta_h - \delta_s$.

(iii) $\partial_2 = [\delta_h, \overline{\delta_h}]$.

(iv) $\partial_3 = \frac{1}{2}\left([\delta_h, [\partial_1, \overline{\delta_h}]] - [\delta_h, \partial_2] - [\overline{\delta_h}, \partial_2]\right)$.

(v) $\partial_4 = \frac{1}{6}\left[\delta_h, [\partial_1, [\partial_1, \overline{\delta_h}]]\right] - \frac{1}{6}\left[\overline{\delta_h}, [\delta_h, [\partial_1, \overline{\delta_h}]]\right] + \frac{1}{6}\left[\partial_1, [\partial_2, \overline{\delta_h}]\right] + \frac{1}{3}[\partial_3, \delta_h] + \frac{1}{3}[\partial_3, \overline{\delta_h}]$.

Proof. Since both sides of each equation are elements in $\mathrm{Der}(\mathfrak{h})$, it is enough to check that the images of x and y coincide. This is a routine computation. ∎

5 Relation to Derivation Relations

In this section, we present a conjectural formula which shows that the derivation relations is a consequence of the regularized double shuffle relations. We give some results in favor of the conjecture. In particular, the "sum formula" is a consequence of the regularized double shuffle relations.

Definition 19 *For each integer $m \geq 1$, define a $\mathbf{Q}$-linear map $\theta_m : \mathfrak{h} \to \mathfrak{h}$ by*

$$\theta_m(w) := (-1)^m \mathrm{reg}(y^m * w - y^m ш w) \quad (w \in \mathfrak{h}).$$

Set $\theta_0 = 1$ (the identity map).

By Theorem 9, we have $\theta_m(w_0) \in \mathrm{Ker}\,\widehat{\zeta}$ for $w_0 \in \mathfrak{h}^0$. This is the "regularized double shuffle relation with $\zeta(\underbrace{1, 1, \dots, 1}_{m})$". Note that $\theta_m(w) = (-1)^m \mathrm{reg}(y^m * w)$, since $\mathrm{reg}(y^m ш w) = \mathrm{reg}(y^m) ш \,\mathrm{reg}(w) = 0$ by Proposition 8 (ii).

The following theorem shows that the sum formula for MZVs, which states that the sum of all MZVs of fixed weight and depth is equal to the Riemann zeta value of that weight, can be deduced from the regularized double shuffle relations.

Theorem 20 *Denote by $S(k, m)$ the sum of all monomials in $\mathfrak{h}^0$ of weight k and depth m. For any k and m with $k > m + 1 \geq 2$, we have*

$$\theta_m(x^{k-m-1}y) = S(k, m+1) - S(k, m).$$

This shows that the sum of all multiple zeta values of fixed weight and depth is independent of depth, hence is equal to the Riemann zeta value.

Proof. The harmonic product $y^m * x^{k-m-1}y$, which corresponds to $\zeta(\underbrace{1, 1, \dots, 1}_{m})\zeta(k-m)$, is easily computed as

$$y^m * x^{k-m-1}y = \sum_{i=0}^{m} y^i x^{k-m-1} y^{m+1-i} + \sum_{j=0}^{m-1} y^j x^{k-m} y^{m-j}.$$

By Proposition 8 (ii),

$$\mathrm{reg}(y^m * x^{k-m-1}y)$$

$$
\begin{aligned}
&= \sum_{i=0}^{m}(-1)^i x(y^i ш x^{k-m-2}y^{m+1-i}) + \sum_{j=0}^{m-1}(-1)^j x(y^j ш x^{k-m-1}y^{m-j}) \\
&= x^{k-m-1}y^{m+1} + \sum_{i=1}^{m}(-1)^i x\left\{(y^i ш x^{k-m-2}y^{m-i})y + (y^{i-1} ш x^{k-m-2}y^{m+1-i})y\right\} \\
&\quad + x^{k-m}y^m + \sum_{j=1}^{m-1}(-1)^j x\left\{(y^j ш x^{k-m-1}y^{m-1-j})y + (y^{j-1} ш x^{k-m-1}y^{m-j})y\right\} \\
&= \sum_{i=0}^{m}(-1)^i x(y^i ш x^{k-m-2}y^{m-i})y + \sum_{i=0}^{m-1}(-1)^{i+1} x(y^i ш x^{k-m-2}y^{m-i})y \\
&\quad + \sum_{j=0}^{m-1}(-1)^j x(y^j ш x^{k-m-1}y^{m-1-j})y + \sum_{j=0}^{m-2}(-1)^{j+1} x(y^j ш x^{k-m-1}y^{m-1-j})y \\
&= (-1)^m x(y^m ш x^{k-m-2})y + (-1)^{m-1} x(y^{m-1} ш x^{k-m-1})y.
\end{aligned}
$$

We therefore have

$$
\begin{aligned}
\theta_m(x^{k-m-1}y) &= x(y^m ш x^{k-m-2})y - x(y^{m-1} ш x^{k-m-1})y \\
&= S(k, m+1) - S(k, m).
\end{aligned}
$$

∎

The sum formula is a special case of Ohno's theorem. Through an attempt of understanding Ohno's theorem in the light of double shuffle relations, we were led to the following conjecture. Put $\widehat{\mathfrak{h}}^0 = \mathbf{Q} + x\widehat{\mathfrak{h}}y$.

Conjecture *On* $\widehat{\mathfrak{h}}^0$,

$$
\exp\left(\sum_{n=1}^{\infty} \frac{\partial_n}{n}\right) = \sum_{m=0}^{\infty} \theta_m.
$$

Put $\Delta = \exp(\sum_{n=1}^{\infty} \frac{\partial_n}{n})$ and $\Theta = \sum_{m=0}^{\infty} \theta_m$. We can at least show that the Δ and Θ agree on the monomials which correspond to the Riemann zeta values, including $y (\leftrightarrow \zeta(1))$.

Proposition 21

$$
\Delta(x^k y) = \Theta(x^k y), \ \forall k \geq 0.
$$

Proof. First we prove $\Delta(y) = \Theta(y)$. We know from Proposition 6 (and its proof) that $\Delta(y) = y - xy(1-y)^{-1}$. Since for $m \geq 1$

$$
\begin{aligned}
\theta_m(y) &= (-1)^m \mathrm{reg}(y^m * y) \\
&= (-1)^m \mathrm{reg}((m+1)y^{m+1} + \sum_{i=0}^{m-1} y^i x y^{m-i})
\end{aligned}
$$

$$
\begin{aligned}
&= (-1)^m \sum_{i=0}^{m-1} (-1)^i x (y^i ш\, y^{m-i}) \\
&= (-1)^m \sum_{i=0}^{m-1} (-1)^i x \binom{m}{i} y^m \\
&= (-1)^m (-(-1)^m x y^m) \\
&= -xy^m,
\end{aligned}
$$

$$\Theta(y) = \sum_{m=0}^{\infty} \theta_m(y) = y - xy(1-y)^{-1}.$$

Next assume $k \geq 1$. As was shown in the proof of Theorem 20,

$$\theta_m(x^k y) = x(y^m ш\, x^{k-1})y - x(y^{m-1} ш\, x^k)y$$

for $m, k \geq 1$. Hence

$$\Theta(x^k y) = x((1-y)^{-1} ш\, x^{k-1})y - x((1-y)^{-1} ш\, x^k)y.$$

On the other hand, since Δ is a homomorphism with respect to the concatenation product and we know that $\Delta(y) = y - xy(1-y)^{-1}$, $\Delta(x) = \Delta(x+y-y) = x + y - (y - xy(1-y)^{-1}) = x(1-y)^{-1}$, we have

$$\Delta(x^k y) = \underbrace{x(1-y)^{-1} x(1-y)^{-1} \cdots x(1-y)^{-1}}_{k} (y - xy(1-y)^{-1}).$$

In view of the lemma below, this is equal to $\Theta(x^k y)$.

Lemma 22 *For $k \geq 0$,*

$$(1-y)^{-1} ш\, x^k = (1-y)^{-1} \underbrace{x(1-y)^{-1} x(1-y)^{-1} \cdots x(1-y)^{-1}}_{k}.$$

Proof.

$$
\begin{aligned}
\sum_{m=0}^{\infty} y^m ш\, x^k &= \sum_{m=0}^{\infty} \sum_{\substack{i_1, i_2, \ldots, i_{k+1} \geq 0 \\ i_1 + i_2 + \cdots + i_{k+1} = m}} y^{i_1} x y^{i_2} x \cdots x y^{i_{k+1}} \\
&= \sum_{i_1, i_2, \ldots, i_{k+1} \geq 0} y^{i_1} x y^{i_2} x \cdots x y^{i_{k+1}} \\
&= (1-y)^{-1} \underbrace{x(1-y)^{-1} x(1-y)^{-1} \cdots x(1-y)^{-1}}_{k}.
\end{aligned}
$$

∎

Remark (i) Besides the conjecture, we also checked by computer that, up to weight 13, the linear relations obtained by Zagier's theorem are equivalent to those obtained by the derivation relations. However, we could not find an exact formula connecting the two relations.

(ii) If the conjecture is true, then θ_m's commute with each other because of Lemma 3. But we could not prove this.

(iii) It seems that Θ and Δ do *not* coincide on the whole $\mathfrak{h}$ (although $\Theta(x) = \Delta(x)$ and $\Theta(y) = \Delta(y)$). For example, $\Theta(y^2) \neq \Theta(y)^2$ whereas $\Delta(y^2) = \Delta(y)^2$ since Δ is an automorphism on $\mathfrak{h}$. How should we understand this?

6 Formal KZ associator

We shall define and study an element $\widehat{\Phi}(X,Y)$ in $\mathfrak{h}_{sh}\langle\langle X,Y\rangle\rangle$, the non-commutative formal power series algebra over the shuffle algebra $\mathfrak{h}_{sh}$. Here, X and Y are non-commuting indeterminates, commute with elements in $\mathfrak{h}_{sh}$, and the multiplication of coefficients in $\mathfrak{h}_{sh}$ is the shuffle product $ш$.

We denote by $\{x,y\}^*$ (resp. $\{X,Y\}^*$) the set of all words (including empty word regarded as 1) in x and y (resp. X and Y). For $w \in \{x,y\}^*$, let $\mathrm{cap}(w) \in \{X,Y\}^*$ be the corresponding "capitalization" of w. For example, $\mathrm{cap}(xy) = XY, \mathrm{cap}(x^2y^3x) = X^2Y^3X$, etc. We set $\mathrm{cap}(1) = 1$.

We recall briefly the definition of Drinfeld's KZ associator [2]. For more detail, see *e.g.*, [6, Ch. XIX].

Consider the linear differential equation

$$G'(z) = \left(\frac{X}{z} + \frac{Y}{z-1}\right)G(z) \tag{11}$$

and its unique solutions $G_0(z)$ and $G_1(z)$ such that

$$G_0(z) \sim z^X \ (z \to 0) \quad \text{and} \quad G_1(z) \sim (1-z)^Y \ (z \to 1).$$

The Drinfeld KZ associator $\Phi_{KZ}(X,Y)$ is an element in $\mathbf{R}\langle\langle X,Y\rangle\rangle$ defined by

$$\Phi_{KZ}(X,Y) = G_1(z)^{-1}G_0(z).$$

Definition 23 *The formal KZ associator $\widehat{\Phi}(X,Y)$ is an element in $\mathfrak{h}_{sh}\langle\langle X,Y\rangle\rangle$ defined by*

$$\widehat{\Phi}(X,Y) = \exp_{sh}(-yY) \cdot \sum_{\substack{w\in\{x,y\}^* \\ W\in\{X,Y\}^* \\ W=\mathrm{cap}(w)}} wW \cdot \exp_{sh}(-xX),$$

where $\exp_{sh}(-yY) = \sum_{n=0}^{\infty}(-1)^n y^{ш n}\frac{Y^n}{n!}$, $y^{ш n} = \underbrace{y ш y ш \cdots ш y}_{n}$ *and similarly for* $\exp_{sh}(-xX)$.

Remark Since $(\underbrace{y ш y ш \cdots ш y}_{i})/i! = y^i$, $(\underbrace{x ш x ш \cdots ш x}_{j})/j! = x^j$, this can also be written as

$$\widehat{\Phi}(X,Y) = \sum_{i=0}^{\infty}(-1)^i y^i Y^i \cdot \sum_{\substack{w\in\{x,y\}^* \\ W\in\{X,Y\}^* \\ W=\mathrm{cap}(w)}} wW \cdot \sum_{j=0}^{\infty}(-1)^j x^j X^j.$$

Proposition 24 (i) *The coefficient of* $W = \mathrm{cap}(w)$ *of* $\widehat{\Phi}(X,Y)$ *is given by* $\mathrm{reg}(w)$;

$$\widehat{\Phi}(X,Y) = \sum_{\substack{w\in\{x,y\}^* \\ W\in\{X,Y\}^* \\ W=\mathrm{cap}(w)}} \mathrm{reg}(w)W,$$

so we have

$$\widehat{\Phi}(X,Y) \in \mathfrak{h}^0_{sh}\langle\langle X,Y\rangle\rangle.$$

(ii) *Let* $\widehat{\zeta}$ *be the map* $\mathfrak{h}^0_{sh}\langle\langle X,Y\rangle\rangle \to \mathbf{R}\langle\langle X,Y\rangle\rangle$ *which is obtained by extending the evaluation map* $\widehat{\zeta} : \mathfrak{h}^0 \to \mathbf{R}$ *coefficient-wise. Then we have*

$$\widehat{\zeta}(\widehat{\Phi}(X,Y)) = \Phi_{KZ}(X,-Y).$$

Proof. (i) is immediate from the definition of $\widehat{\Phi}(X,Y)$, the above remark, and Proposition 8 (i).

(ii) For a real number a such that $0 < a < 1$, let $G_a(z)$ be the unique solution of (11) such that $G_a(a) = 1$. Then ([6, Lemma XIX.6.3])

$$\Phi_{KZ}(X,-Y) = \lim_{a\to 0} a^Y G_a(1-a)a^X.$$

From this, we have

$$\Phi_{KZ}(X,-Y) = \lim_{a\to 0}(\frac{a}{1-a})^Y G_a(1-a)(\frac{a}{1-a})^X.$$

Each factor on the right has an expression as an iterated integrals as follows. First,

$$\begin{aligned}
(\frac{a}{1-a})^Y &= \exp(\log(\frac{a}{1-a})Y) \\
&= \exp(-\int_a^{1-a}\frac{dt}{1-t}Y) \\
&= \sum_{i=0}^{\infty}\frac{(-1)^i}{i!}\left(\int_a^{1-a}\frac{dt}{1-t}\right)^i Y^i \\
&= \sum_{i=0}^{\infty}(-1)^i\left(\int\cdots\int_{1-a>t_1>t_2>\cdots>t_i>a}\frac{dt_1}{1-t_1}\frac{dt_2}{1-t_2}\cdots\frac{dt_i}{1-t_i}\right)Y^i
\end{aligned}$$

and

$$\begin{aligned}(\frac{a}{1-a})^X &= \exp(\log(\frac{a}{1-a})X) \\ &= \exp(-\int_a^{1-a}\frac{dt}{t}X) \\ &= \sum_{i=0}^{\infty}\frac{(-1)^i}{i!}\left(\int_a^{1-a}\frac{dt}{t}\right)^i X^i \\ &= \sum_{i=0}^{\infty}(-1)^i\left(\int\cdots\int_{1-a>t_1>t_2>\cdots>t_i>a}\frac{dt_1}{t_1}\frac{dt_2}{t_2}\cdots\frac{dt_i}{t_i}\right)X^i.\end{aligned}$$

For each word $w = u_1u_2\cdots u_k \in \{x,y\}^*$, let $\Omega(w)$ be the differential form $\frac{dt_1}{A_1(t_1)}\frac{dt_2}{A_2(t_2)}\cdots\frac{dt_k}{A_k(t_k)}$ where $A_i(t)$ is t or $1-t$ according as u_i is x or y, and denote by $\int_a^{1-a}\Omega(w)$ the multiple integral

$$\int\cdots\int_{1-a>t_1>t_2>\cdots>t_k>a}\Omega(w).$$

The above formulas can then be written as

$$(\frac{a}{1-a})^Y = \sum_{i=0}^{\infty}(-1)^i\left(\int_a^{1-a}\Omega(y^i)\right)Y^i$$

and

$$(\frac{a}{1-a})^X = \sum_{j=0}^{\infty}(-1)^j\left(\int_a^{1-a}\Omega(x^j)\right)X^j.$$

As for $G_a(1-a)$, we have by [6, Ch. XIX (6.8)]

$$G_a(1-a) = 1 + \sum_{\substack{w\in\{x,y\}^*\setminus\{1\} \\ W\in\{X,Y\}^* \\ W=\mathrm{cap}(w)}}\left(\int_a^{1-a}\Omega(w)\right)W.$$

The assertion (ii) then follows from the shuffle product of iterated integrals and Proposition 8 (i), since $\mathrm{reg}(w) \in \mathfrak{h}^0$ so that we can let $a \to 0$ and obtain

$$\lim_{a\to 0} a^Y G_a(1-a)a^X = \widehat{\zeta}(\widehat{\Phi}(X,Y)).$$

∎

Remark Zagier's theorem as formulated in the last paragraph of §3 may also be stated as a relation of two formal "associator-like" objects. Namely, let

$$\widehat{\Phi}^1_{sh}(X,Y) = \exp_{sh}(-yY)\cdot\sum_{\substack{w\in\{x,y\}^*\cap\mathfrak{h}^1 \\ W=\mathrm{cap}(w)}} wW \in \mathfrak{h}^0_{sh}\langle\langle X,Y\rangle\rangle$$

and

$$\widehat{\Phi}^1_{har}(X,Y) = \exp_{har}(-yY)\cdot \sum_{\substack{w\in\{x,y\}^*\cap\mathfrak{h}^1\\ W=\mathrm{cap}(w)}} wW \in \mathfrak{h}^0_{har}\langle\langle X,Y\rangle\rangle.$$

Here, $\exp_{har}(-yY) = \sum_{n=0}^{\infty}(-1)^n y^{*n}\frac{Y^n}{n!}$. Then, we have

$$\widehat{\zeta}(\widehat{\Phi}^1_{sh}(X,Y)) = \widehat{\zeta}\left(\exp_{har}\left(\sum_{r=2}^{\infty}(-1)^r\frac{x^{r-1}y}{r}Y^r\right)\cdot\widehat{\Phi}^1_{har}(X,Y)\right).$$

Questions (i) Let $\mathfrak{a}$ be the subspace of $\mathfrak{h}^0$ generated by all regularized double shuffle relations $\mathrm{reg}(w * w_0 - w ⧢ w_0)$, $\forall w \in \mathfrak{h}^1$, $\forall w_0 \in \mathfrak{h}^0$. Does $\mathfrak{a}$ form an ideal of $\mathfrak{h}^0_{sh}$? If so, put $\mathfrak{h}_{dsh} = \mathfrak{h}^0_{sh}/\mathfrak{a}$. Does the image of $\widehat{\Phi}(X,-Y)$ in $\mathfrak{h}_{dsh}\langle\langle X,Y\rangle\rangle$ satisfy 2, 3 and 5 cycle relations of KZ associator? The image in $(\mathfrak{h}^0_{sh}/\mathrm{Ker}\,\widehat{\zeta})\langle\langle X,Y\rangle\rangle$ is identified with $\Phi_{KZ}(X,Y)$ and does indeed satisfy 2, 3 and 5 cycle relations.

(ii) Conversely, let $\mathfrak{b}$ be the minimal ideal of $\mathfrak{h}^0_{sh}$ such that the image of the formal associator $\widehat{\Phi}(X,-Y)$ in $(\mathfrak{h}^0_{sh}/\mathfrak{b})\langle\langle X,Y\rangle\rangle$ satisfies 2, 3 and 5 cycle relations. Does $\mathfrak{b}$ coincide with $\mathrm{Ker}\,\widehat{\zeta}$, or the space of regularized double shuffle relations?

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