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Abstract

We study the depth filtration on multiple zeta values, on the motivic Galois group of mixed Tate motives over $\mathbb{Z}$ and on the Grothendieck–Teichmüller group, and its relation to modular forms. Using period polynomials for cusp forms for $\mathrm{SL}_2(\mathbb{Z})$, we construct an explicit Lie algebra of solutions to the linearized double shuffle equations, which gives a conjectural description of all identities between multiple zeta values modulo $\zeta(2)$ and modulo lower depth. We formulate a single conjecture about the homology of this Lie algebra which implies conjectures due to Broadhurst and Kreimer, Racinet, Zagier, and Drinfeld on the structure of multiple zeta values and on the Grothendieck–Teichmüller Lie algebra.

1. Introduction

We begin by motivating the results of this paper from two apparently different, but in fact equivalent, perspectives.

1.1 Depth filtration on multiple zeta values

Multiple zeta values are defined for integers $n_1, \ldots, n_{r-1} \geq 1$ and $n_r \geq 2$ by

$$\zeta(n_1, \ldots, n_r) = \sum_{1 \leq k_1 < \cdots < k_r} \frac{1}{k_1^{n_1} \ldots k_r^{n_r}}.$$

Their weight is the quantity $n_1 + \cdots + n_r$, and their depth is the number of indices r. Relations between multiple zeta values of depth 2 were first studied by Euler. Let $\mathcal{Z}_N$ denote the $\mathbb{Q}$-vector space spanned by multiple zeta values in weight N. Zagier conjectured, firstly, that the space $\mathcal{Z}$ of multiple zeta values is isomorphic to the direct sum of the $\mathcal{Z}_N$ (in other words, the weight is a grading), and secondly, that the dimension of $\mathcal{Z}_N$ can be expressed using the generating series

$$\sum_{N \geq 0} \dim_{\mathbb{Q}} (\mathcal{Z}_N) s^N = \frac{1}{1 - s^2 - s^3}. \tag{1.1}$$

Using the theory [Lev93, DG05] of mixed Tate motives over $\mathbb{Z}$, Goncharov [Gon01a] and Terasoma [Ter02] independently showed that $\dim_{\mathbb{Q}} \mathcal{Z}_N$ is bounded above by the coefficient of s^N in the

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right-hand side of (1.1). Furthermore, if one replaces $\mathcal{Z}_N$ with the $\mathbb{Q}$-vector space of motivic multiple zeta values $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$ of weight N, then (1.1) is a theorem [Bro12, Del13]. The rational function on the right-hand side of (1.1) can be interpreted as follows: it is the Poincaré series of the free graded module, generated by $\zeta^{\mathfrak{m}}(2n)$ for $n \geq 1$, over the graded dual of the universal enveloping algebra of the Lie algebra of the category of mixed Tate motives over $\mathbb{Z}$, which is free with one generator in every odd degree ≤ -3 (see [DG05, Del13] for further details).

Based on numerical experiments, Broadhurst and Kreimer [BK97] formulated a fascinating and more refined conjecture which takes into account the depth. The depth, by contrast with the conjectural properties of the weight, is only a filtration, and not a grading. Let $\mathcal{Z}_{N,d}$ denote the $\mathbb{Q}$-vector space spanned by multiple zeta values in weight N and depth d, modulo multiple zeta values of weight N and strictly lower depth. They propose that

$$\sum_{N,d \geq 0} \dim_{\mathbb{Q}} (\mathcal{Z}_{N,d}) s^N t^d = \frac{1 + \mathbb{E}(s)t}{1 - \mathbb{O}(s)t + \mathbb{S}(s)t^2 - \mathbb{S}(s)t^4}, \tag{1.2}$$

where, using the notation from [IKZ06, Appendix],

$$\mathbb{E}(s) = \frac{s^2}{1-s^2}, \quad \mathbb{O}(s) = \frac{s^3}{1-s^2}, \quad \mathbb{S}(s) = \frac{s^{12}}{(1-s^4)(1-s^6)}. \tag{1.3}$$

Formula (1.2) specializes to the statement (1.1) upon setting $t = 1$.

The meaning of this conjecture is still mysterious, but one goal of this paper is to offer a homological interpretation of (1.2). The series $\mathbb{E}(s)$ and $\mathbb{O}(s)$ are the generating series for the dimensions of the spaces of even and odd single zeta values respectively, and $\mathbb{S}(s)$ is the generating series for the dimensions of the space of cusp forms for the full modular group $\mathrm{SL}_2(\mathbb{Z})$. The first prediction of (1.2), due to the presence of a non-trivial coefficient of t^2 in the denominator of the right-hand side, is the existence of an extra relation between double zeta values of even weight for every cusp form, modulo multiple zeta values of lower depth (single zeta values). These relations have indeed been shown to exist and are well understood by the work of Gangl *et al.* [GKZ06], who exhibited an infinite family of such relations. The smallest one corresponds to the Ramanujan cusp form of weight 12:

$$28\,\zeta(3,9) + 150\,\zeta(5,7) + 168\,\zeta(7,5) = \frac{5197}{691}\zeta(12). \tag{1.4}$$

The coefficients in this and all such equations can be related to period polynomials for cusp forms, or equivalently, to group cocycles for $\mathrm{SL}_2(\mathbb{Z})$. Furthermore, a geometric mechanism for these relations is by now fairly well understood [Bro14b].

The situation in higher depths remains very unclear. It is known by work of Zagier [Zag93] and Goncharov [Gon01b] that (1.2) is true (in a suitable setting, i.e. for solutions to the double shuffle equations as discussed below) in depths 2 and 3, respectively. Nevertheless, the presence of the term in t^4 in the right-hand side of (1.2) suggests a new phenomenon in depth 4. If we interpret the right-hand side of (1.2) in terms of the Poincaré series of a depth-graded version of the Lie algebra of the category of mixed Tate motives over $\mathbb{Z}$, the term in t^4 suggests the existence of *new generators* in this Lie algebra in depth 4, corresponding to cusp forms for the full modular group.

In this paper we supply candidates for these 'exceptional' generators by constructing them explicitly out of period polynomials of cusp forms. As a result, we can formulate a much more precise conjecture than (1.2) which predicts not only the dimensions of the spaces of multiple

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zeta values in all weights and depths, but also their relations and modulo lower depths. In order to get some sense of these exceptional generators, consider the first one, which occurs in depth 4 and weight 12. It turns out that all multiple zeta values in weight 12 and depth 4 are proportional to a single element $\zeta(1,1,2,8)$ modulo terms of lower depth and products, for example,

$$\zeta(4,3,3,2) \equiv 116\,\zeta(1,1,2,8).$$

The exceptional generator corresponding to the Ramanujan cusp form Δ annihilates every such relation, and therefore gives an interpretation of the coefficients (in this case, the number 116) in terms of ratios of critical values of the L-function of Δ.

1.2 The projective line minus three points

Let $\mathcal{G}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})} = \mathrm{Aut}^{\otimes}_{\mathcal{MT}(\mathbb{Z})}(\omega_{\mathrm{dR}})$ denote the motivic Galois group of the Tannakian category $\mathcal{MT}(\mathbb{Z})$ of mixed Tate motives over the integers [DG05], and let $\mathcal{U}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})} \leq \mathcal{G}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})}$ denote its unipotent radical. One has a canonical isomorphism $\mathcal{G}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})} = \mathcal{U}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})} \rtimes \mathbb{G}_m$. Let

$${}_0\Pi_0 = \pi_1^{\mathrm{dR}}(\mathbb{P}^1\backslash\{0,1,\infty\}, \vec{1}_0) \quad \text{and} \quad {}_0\Pi_1 = \pi_1^{\mathrm{dR}}(\mathbb{P}^1\backslash\{0,1,\infty\}, \vec{1}_0, -\vec{1}_1)$$

denote the de Rham fundamental group (respectively, torsor of paths) at a tangential base point at 0 (respectively, between tangential basepoints at 0 and 1) [Del89]. The latter is a torsor over the former, via composition[1] of paths ${}_0\Pi_0 \times {}_0\Pi_1 \to {}_0\Pi_1$. Since ${}_0\Pi_0, {}_0\Pi_1$ are the de Rham realizations of (pro)-objects in the category of mixed Tate motives over $\mathbb{Z}$, the group $\mathcal{G}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})}$ acts upon them, and there is a canonical representation

$$\mathcal{G}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})} \longrightarrow \mathrm{Aut}\big({}_0\Pi_0 \times {}_0\Pi_1\big),$$

where the group of automorphisms on the right denotes those automorphisms which respect the structure ${}_0\Pi_0 \times {}_0\Pi_x \to {}_0\Pi_x$ for $x \in \{0,1\}$. This action is the motivic version of the outer action of the absolute Galois group $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$ on the pro-ℓ completion of the fundamental group of X which was first studied extensively by Deligne, Drinfeld, and Ihara [Del13, Dri90, Iha02]. Deligne conjectured that this action is faithful, or equivalently, that the motivic torsor of paths on X generates the category $\mathcal{MT}(\mathbb{Z})$, which was shown in [Bro12, Del13]. The graded Lie algebra[2] of ${}_0\Pi_0$ is the free graded Lie algebra $\mathbb{L}(e_0, e_1)$ on two generators e_0, e_1. Therefore, the infinitesimal version of the action of $\mathcal{U}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})}$ on ${}_0\Pi_0$ gives a very concrete way to study the motivic Galois group, or equivalently, its graded Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ together with its representation:

$$\mathfrak{g}^{\mathfrak{m}} := \mathrm{Lie}\,\mathcal{U}^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})} \longrightarrow \mathrm{Der}\,\mathrm{Lie}\,{}_0\Pi_0 = \mathrm{Der}\,\mathbb{L}(e_0, e_1).$$

One shows that the image of $\mathfrak{g}^{\mathfrak{m}}$ lies in the Lie subalgebra of derivations which are in the image of the linear map

$$\mathbb{L}(e_0, e_1) \mapsto \mathrm{Der}\,\mathbb{L}(e_0, e_1)$$

$$f \mapsto D_f,$$

[1] We use the topologist's convention: $\alpha\beta$ denotes the path α followed by the path β.

[2] Throughout this paper, the notation Lie will denote a (weight)-graded Lie algebra, that is, a Lie algebra graded for the action of $\mathbb{G}_m$.

where $D_f(e_0) = 0$ and $D_f(e_1) = [f, e_1]$. One can equip $\mathbb{L}(e_0, e_1)$ with a new Lie algebra structure $\{\,,\}$, called the Ihara bracket, such that the previous map becomes a morphism of Lie algebras (i.e. $D_{\{f,g\}} = [D_f, D_g]$), where the bracket on the right is the usual Lie bracket on derivations. Let us denote the graded vector space $\mathbb{L}(e_0, e_1)$ together with this new Lie algebra structure by $\mathfrak{g} := (\mathbb{L}(e_0, e_1), \{\,,\})$.

One obtains from all this a canonical embedding of the motivic Lie algebra

$$\mathfrak{g}^{\mathfrak{m}} \subset \mathfrak{g}.$$

By abuse of notation, we shall identify $\mathfrak{g}^{\mathfrak{m}}$ with its image in $\mathfrak{g}$. The injectivity of $\mathfrak{g}^{\mathfrak{m}} \to \mathfrak{g}$ follows from [Bro12].

A major problem is to describe this Lie algebra as precisely as possible. We know that it has generators called 'zeta elements' for every $n \geq 1$:

$$\sigma_{2n+1} = (\mathrm{ad}\, e_0)^{2n}\, e_1 + (\text{terms of degree } \geq 2 \text{ in } e_1)$$

but they are not canonical[3] (e.g. σ_{11} is only well defined up to addition of rational multiples of $\{\sigma_3, \{\sigma_5, \sigma_3\}\}$). Deligne's conjecture in its originally stated form was that the ℓ-adic versions of the σ_{2n+1}, which are elements in a certain Lie algebra constructed out of $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$, form a free Lie algebra for the Ihara bracket.

Theorem 1.1 [Bro12]. *The graded Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ is a free Lie algebra on (some choice of) generators σ_{2n+1} in each degree $-(2n+1)$ for $n \geq 1$.*

Only the classes $[\sigma_{2n+1}]$ in the abelianization $(\mathfrak{g}^{\mathfrak{m}})^{\mathrm{ab}} = \mathfrak{g}^{\mathfrak{m}}/\{\mathfrak{g}^{\mathfrak{m}}, \mathfrak{g}^{\mathfrak{m}}\}$ are canonical. Since $H_1(\mathfrak{g}^{\mathfrak{m}}; \mathbb{Q}) = (\mathfrak{g}^{\mathfrak{m}})^{\mathrm{ab}}$, one can rephrase the previous theorem by saying that

$$\begin{aligned} H_1(\mathfrak{g}^{\mathfrak{m}}; \mathbb{Q}) &\cong \bigoplus_{n\geq 1} [\sigma_{2n+1}]\mathbb{Q}, \\ H_i(\mathfrak{g}^{\mathfrak{m}}; \mathbb{Q}) &= 0, \quad \text{for } i \geq 2. \end{aligned} \tag{1.5}$$

The abstract structure of the Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ is therefore very simple, but the information about linear relations between multiple zeta values is encoded in the coefficients of the generators σ_{2n+1}, which are not known explicitly. In this paper we study the associated graded version $\mathfrak{dg}^{\mathfrak{m}}$ of this Lie algebra for a filtration called the depth, which is related to the depth filtration on multiple zeta values. By contrast with the case of $\mathfrak{g}^{\mathfrak{m}}$, we will provide an explicit conjectural description of all the generators of $\mathfrak{dg}^{\mathfrak{m}}$. It is not a free Lie algebra, but a little more complicated.

1.3 Depth filtration on the motivic Lie algebra

As defined in [DG05], the depth filtration is induced geometrically by the inclusion $\mathbb{P}^1\backslash\{0, 1, \infty\} \subset \mathbb{G}_m$ and is the decreasing filtration $\mathfrak{D}$ on $\mathbb{L}(e_0, e_1)$, where $\mathfrak{D}^r$ consists of Lie brackets containing at least r occurrences of the letter e_1. It is preserved by the Ihara bracket $\{\,,\}$, and therefore defines a filtration on $\mathfrak{g}$. One defines the depth filtration $\mathfrak{D}^r\mathfrak{g}^{\mathfrak{m}}$ to be the induced filtration. An element in $\mathfrak{g}^{\mathfrak{m}}$ lies in $\mathfrak{D}^r\mathfrak{g}^{\mathfrak{m}}$ if and only if the corresponding derivation of $\mathrm{Lie}\,{}_0\Pi_0 = \mathbb{L}(e_0, e_1)$ sends

[3] In fact, one can define canonical generators σ_{2n+1} to be the coefficient of $\zeta^{\mathfrak{m}}(3, 2, \ldots, 2)$, with $n-1$ twos, in a motivic Drinfeld associator $\Phi^{\mathfrak{m}} = \sum_w \zeta^{\mathfrak{m}}(w)w$. However, this definition is not explicit and most of the coefficients of σ_{2n+1} defined in this way are not known.

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$\mathfrak{D}^s$ to $\mathfrak{D}^{s+r}$ for all s. This makes the motivic nature of $\mathfrak{D}$ clear since the σ_{2n+1} increase the depth by at least 1.

We consider the associated graded Lie algebra:

$$\mathfrak{dg}^{\mathfrak{m}} = \mathrm{gr}_{\mathfrak{D}}\mathfrak{g}^{\mathfrak{m}}.$$

It is bigraded by weight and depth: the depth will be indicated by a subscript, thus $\mathfrak{dg}^{\mathfrak{m}}_r = \mathrm{gr}^r_{\mathfrak{D}}\mathfrak{g}^{\mathfrak{m}}$. We identify $\mathfrak{dg}^{\mathfrak{m}}$ with a Lie subalgebra of $\mathrm{gr}_{\mathfrak{D}}\mathfrak{g}$ which as a bigraded vector space is identified with $\mathbb{L}(e_0, e_1)$. Note that, in fact, the Ihara bracket $\{\, ,\}$ respects the depth grading on the free Lie algebra $\mathbb{L}(e_0, e_1)$, so the Lie bracket on $\mathrm{gr}_{\mathfrak{D}}\mathfrak{g}$ is given by the identical formula to that for $\{\, ,\}$.

In depth 1, $\mathfrak{dg}^{\mathfrak{m}}$ inherits canonical 'zeta' generators which are the images of σ_{2n+1}:

$$\bar{\sigma}_{2n+1} = (\mathrm{ad}\, e_0)^{2n} e_1 \in \mathfrak{dg}^{\mathfrak{m}}_1. \tag{1.6}$$

Ihara discovered, astonishingly, that in the depth-graded Lie algebra the generators $\bar{\sigma}_{2n+1}$ are not free. The first relation occurs in weight 12:

$$\{\bar{\sigma}_3, \bar{\sigma}_9\} - 3\{\bar{\sigma}_5, \bar{\sigma}_7\} = 0. \tag{1.7}$$

In order to reconcile this relation with the freeness theorem (Theorem 1.1), there must exist an extra generator in $\mathfrak{dg}^{\mathfrak{m}}$ in weight 12 to compensate for it: the new generator is given by the lowest depth part of $\{\sigma_3, \sigma_9\} - 3\{\sigma_5, \sigma_7\}$, which is in depth ≥ 4. Exceptional generators such as these (but defined in a direct and somewhat different manner) are one of the main objects of study of this paper.

The general quadratic relations between the $\bar{\sigma}_{2n+1}$ have been known explicitly for some time [IT93, Sch06, Gon05, GKZ06] and will be re-derived as an immediate consequence of the formalism we introduce below. To describe them, let $V_n = \bigoplus_{i+j=n} \mathbb{Q}X^iY^j$ denote the vector space of homogeneous polynomials of degree n in two variables, with its right action of $\mathrm{SL}_2(\mathbb{Z})$. Evaluating cocycles on the matrix $\left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ induces an isomorphism

$$H^1_{\mathrm{cusp}}(\mathrm{SL}_2(\mathbb{Z}), V_{2n-2})^+ \cong \mathsf{S}_{2n},$$

where $+$ denotes invariants under the involution which sends a cocycle $\gamma \mapsto C_\gamma$ to the cocycle $\gamma \mapsto C_{\epsilon\gamma\epsilon^{-1}}\big|_\epsilon$, where $\epsilon = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. One can show that this involution is induced by the action of complex conjugation on $(\mathbb{C}\backslash\mathbb{R})/\mathrm{GL}_2(\mathbb{Z})$. The space $\mathsf{S}_{2n} \subset \mathbb{Q}[X, Y]$ is the space of even-period polynomials: it is the space of antisymmetric homogeneous polynomials $P(X, Y)$ of degree $2n-2$, divisible by Y, satisfying $P(\pm X, \pm Y) = P(X, Y)$ and

$$P(X, Y) + P(X-Y, X) + P(-Y, X-Y) = 0.$$

One shows that the quadratic relations between $\bar{\sigma}_{2i+1}$ in weight $2n+2$ are completely described by period polynomials in S_{2n}:

$$\sum_{i<j} \lambda_{i,j}\{\bar{\sigma}_{2i+1}, \bar{\sigma}_{2j+1}\} = 0 \iff \sum_{i<j} \lambda_{i,j}\big(X^{2i}Y^{2j} - X^{2j}Y^{2i}\big) \in \mathsf{S}_{2n}, \tag{1.8}$$

where $i + j = n$ in both equations. The first goal of this paper is to provide a complete conjectural description of $\mathfrak{dg}^{\mathfrak{m}}$.

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1.4 Results

1.4.1 *Missing generators.* Firstly, we construct the candidate exceptional generators in depth 4 using period polynomials for cusp forms. We define an explicit map

$$\mathsf{e} : H^1_{\mathrm{cusp}}(\mathrm{SL}_2(\mathbb{Z}); V_{2n-2})^+ \longrightarrow \mathfrak{D}^4\mathfrak{g}$$

which, to every even-period polynomial associates a Lie word in two generators e_0, e_1, of degree 4 in e_1. A different source of extra generators in depth 4 are the lowest- depth part of expressions of the form $\sum_{i<j} \lambda_{i,j}\{\sigma_{2i+1}, \sigma_{2j+1}\}$ where the $\lambda_{i,j}$ are as in (1.8) (these expressions have depth ≥ 4) but such generators depend on a choice of generators σ_{2n+1}. A canonical choice of such generators was given in [Bro17a], but the relationship with the elements e, which are introduced in the present paper and defined very differently, is not completely understood. For instance, even if one works modulo commutators, these two possible definitions of generators in depth 4 are related by a non-trivial isomorphism on the space of period polynomials (see §§ 1.4.3, 8.4).

The simplest possible conjecture that one can make is that the depth-graded motivic Lie algebra is generated by the canonical generators $\bar{\sigma}_{2n+1}$ in depth 1, the image of the exceptional map e in depth 4 and subject only to the known quadratic relations between the $\bar{\sigma}_{2n+1}$ in depth 2. This is equivalent to a statement about $H_i(\mathfrak{dg}^{\mathfrak{m}}; \mathbb{Q})$ for $i = 1, 2$, and suggests the following reformulation of the Broadhurst–Kreimer conjecture.

Conjecture 1. The image of e lies in $\mathfrak{dg}^{\mathfrak{m}}$, and

$$\begin{aligned} H_1(\mathfrak{dg}^{\mathfrak{m}}; \mathbb{Q}) &\cong \bigoplus_{n\geq 1} \bar{\sigma}_{2n+1}\mathbb{Q} \oplus \bigoplus_n \mathsf{e}(\mathsf{S}_{2n}), \\ H_2(\mathfrak{dg}^{\mathfrak{m}}; \mathbb{Q}) &\cong \bigoplus_n \mathsf{S}_{2n}, \\ H_i(\mathfrak{dg}^{\mathfrak{m}}; \mathbb{Q}) &= 0, \quad \text{for } i \geq 3. \end{aligned} \tag{1.9}$$

We show in § 10.2 that Conjecture 1 implies the version of (1.2) in which multiple zeta values are replaced by motivic multiple zeta values. This is in turn equivalent to (1.2) if one assumes the period conjecture for mixed Tate motives over $\mathbb{Z}$.

Conjecture 1 describes all relations between depth-graded motivic multiple zeta values (modulo products and $\zeta^{\mathfrak{m}}(2)$). More precisely, consider the ring $\mathcal{H}$ of shuffle-regularized motivic multiple zeta values $\zeta^{\mathfrak{m}}(w)$ where w is a word in $\{e_0, e_1\}$. It is weight-graded, and also has a depth filtration $\mathfrak{D}$, which counts the number of e_1's. Let $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}$ denote the associated graded ring and let $\mathrm{gr}^{\mathfrak{D}}I$ denote its augmentation ideal. Then a linear relation of weight N and depth d of the form

$$\sum_w \lambda_w \, \zeta^{\mathfrak{m}}(w) \equiv 0,$$

where $\lambda_w \in \mathbb{Q}$ and w ranges over words in e_0, e_1 of length N with d letters e_1, holds in the quotient[4] $(\mathrm{gr}^{\mathfrak{D}}\mathcal{H})/((\mathrm{gr}^{\mathfrak{D}}I)^2 + (\zeta^{\mathfrak{m}}(2)))$ if and only if, for all $x \in \mathfrak{dg}^{\mathfrak{m}}_d$ of weight N and depth d of the

[4] This is equal to the depth-graded of the quotient $\mathcal{H}/((I)^2 + (\zeta^{\mathfrak{m}}(2)))$, where I is the augmentation ideal in $\mathcal{H}$. This follows from the fact that (depth graded) motivic multiple zeta values form a polynomial ring (shown in § 4.2) – one can choose a system of motivic multiple zeta values, whose images in the depth-graded are algebraically independent generators for $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}$. Note that there is presently no explicitly known candidate for a family of such generators.

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form $x = \sum_w c_w w$, one has $\sum_w c_w \lambda_w = 0$. Since Conjecture 1 provides an explicit presentation for $\mathfrak{dg}^{\mathfrak{m}}$, it conjecturally describes all such relations between (motivic) depth-graded multiple zeta values (see Example 8.4).

In fact, the formalism developed here enables one to describe all relations between depth-graded motivic multiple zeta values (and not necessarily modulo products or modulo $\zeta^{\mathfrak{m}}(2)$). These are described by the linear forms which vanish not on $\mathfrak{dg}^{\mathfrak{m}}$ but rather on the bigraded right-module over the universal enveloping algebra $\mathcal{U}\mathfrak{dg}^{\mathfrak{m}}$ generated by the depth 1 components of a rational associator $\tau^{(1)}$ (defined in [Bro17a]). This can be made completely explicit: see § 6.7.

1.4.2 *Linearized double shuffle equations.* The main evidence for the previous conjecture comes from the double shuffle equations. It is known that

$$\mathfrak{g}^{\mathfrak{m}} \subset \mathfrak{grt} \subset \mathfrak{dm}_0,$$

where $\mathfrak{grt}$ is Drinfeld's Grothendieck–Teichmüller Lie algebra, and $\mathfrak{dm}_0$ is Racinet's regularized double shuffle Lie algebra, both of which are defined by explicit equations. The inclusion of $\mathfrak{g}^{\mathfrak{m}}$ in $\mathfrak{grt}$ and $\mathfrak{dm}_0$ follow from Theorem 1.1 and results of Drinfeld [Dri90] and Racinet [Rac02], respectively. The inclusion $\mathfrak{grt} \subset \mathfrak{dm}_0$ is due to Furusho [Fur11].

If we pass to the depth-graded Lie algebras, we have

$$\mathfrak{dg}^{\mathfrak{m}} \subset \mathrm{gr}^{\mathfrak{D}}\mathfrak{dm}_0 \subset \mathfrak{ls},$$

where $\mathfrak{ls}$ are the linearized double shuffle equations defined in [IKZ06]. The advantage of these equations are that they are extremely simple to define: $\mathfrak{ls}$ is essentially the intersection of two shuffle algebras. Hitherto, $\mathfrak{ls}$ was studied merely as a vector space, but it turns out, as a consequence of the work of Racinet, that it also inherits a Lie algebra structure for the linearized Ihara bracket. We offer a complete conjectural description of $\mathfrak{ls}$ below.

The first theorem states that the exceptional elements are solutions to the linearized double shuffle equations in depth 4.

Theorem 1.2. *There is an explicit injective linear map*

$$\mathsf{e} : \mathsf{S}_{2n} \longrightarrow \mathfrak{ls}_4. \tag{1.10}$$

The formula for the map e is given in § 8, and associates to every even-period polynomial f a solution e_f of the linearized double shuffle equations. The question of whether the elements e_f are motivic (i.e. whether they lie in the subspace $\mathfrak{dg}^{\mathfrak{m}}$) is open.

Conjecture 2. One has

$$\begin{aligned} H_1(\mathfrak{ls};\mathbb{Q}) &\cong \bigoplus_{n\geq 1} \bar{\sigma}_{2n+1}\mathbb{Q} \oplus \bigoplus_{n} \mathsf{e}(\mathsf{S}_{2n}), \\ H_2(\mathfrak{ls};\mathbb{Q}) &\cong \bigoplus_{n} \mathsf{S}_{2n}, \\ H_i(\mathfrak{ls};\mathbb{Q}) &= 0, \quad \text{for } i \geq 3. \end{aligned} \tag{1.11}$$

This conjecture states, in particular, that $\mathfrak{ls}$ is generated by zeta elements and the exceptional generators in depth 4 subject only to the known quadratic relations between zeta elements. It is at the same time, the simplest and the strongest conjecture that one can formulate.

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It implies several open conjectures about relations between multiple zeta values. For example, it implies: Conjecture 1, and hence the motivic version of the Broadhurst–Kreimer conjecture; the conjecture $\mathfrak{dg}^{\mathfrak{m}} = \mathfrak{ls}$ (which in turn implies a conjecture in [IKZ06]); and the conjectures $\mathfrak{g}^{\mathfrak{m}} = \mathfrak{grt}$ (Drinfeld) and $\mathfrak{g}^{\mathfrak{m}} = \mathfrak{dm}_0$ (Zagier, Racinet). The proofs of these implications use Theorem 1.1 and Furusho's theorem [Fur11] in an essential way. Since the Lie algebra $\mathfrak{ls}$ is defined in a very simple and completely elementary way, the previous conjecture suggest a possibility of seeking a proof of all of the above conjectures intrinsically within the theory of modular forms.

1.4.3 *Discussion.* Note that the vanishing of $H_i(\mathfrak{ls})$ for $i \geq 3$ is equivalent to the vanishing for $i = 3$. This follows from the well-known fact that the vanishing of a Yoneda Ext group causes all higher Ext groups to vanish ([EL16], [Bro17a, Remark 8.6]).

The exceptional elements e satisfy a range of special properties which are studied in §§ 8 and 9. Using these, we can prove that they satisfy no quadratic relations, which provides some meagre evidence in favour of the previous conjectures. We do not know, however, that the e_f are non-trivial in the abelianization of $\mathfrak{ls}$, nor can we presently rule out the existence of relations among the elements of the form

$$\{\mathsf{e}_f, \bar{\sigma}_{2n+1}\} \quad \text{and} \quad \{\bar{\sigma}_{2i_1+1}, \{\bar{\sigma}_{2i_2+1}, \{\bar{\sigma}_{2i_3+1}, \{\bar{\sigma}_{2i_4+1}, \bar{\sigma}_{2i_5+1}\}\}\}\}$$

which are in depth 5 and in weights ≥ 15 (respectively, 17). Relations which are quadratic in the e_f could first occur in weight 28 and depth 8. Viewed from this perspective, the current numerical data in favour of the standard conjectures on multiple zeta values is lacking, since new phenomena could potentially occur in weights and depths beyond the range of current experimentation. Any such phenomena would point to new and fascinating connections between mixed Tate motives over $\mathbb{Z}$ with geometry and arithmetic. Indeed, the methods introduced in this paper should enable one to test the validity of Conjecture 2 to far higher weights than presently known.

The motivic Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ together with its depth filtration $\mathfrak{D}$ naturally gives rise to a spectral sequence (§ 4.5), and the Broadhurst–Kreimer conjecture is equivalent to the statement that this spectral sequence should behave as simply as possible (given the existence of the quadratic relations between $\bar{\sigma}_{2n+1}$); there is only one non-trivial differential,

$$d : \mathsf{S}_{2n} \longrightarrow (\mathfrak{dg}^{\mathfrak{m}}_4)^{\mathrm{ab}}.$$

This is possibly also an argument in favour of Conjecture 1. In [Bro17a] we computed this differential by finding canonical lifts of the zeta elements to depth 3. The relation with the map e is mysterious, although Yasuda has subsequently found a conjectural relation between e and the image of d in the abelianization of $\mathfrak{ls}$ (private correspondence) involving critical values of L-functions of cusp forms. See Example 8.5.

Finally, we investigate the Lie subalgebra of $\mathfrak{dg}^{\mathfrak{m}}$ which is generated only by the elements $\bar{\sigma}_{2n+1}$ (without exceptional elements), and conjecture that it describes the structure of *totally odd* depth-graded motivic multiple zeta values.

1.5 Contents of the paper

In §§ 2–4 we recall some background on the motivic fundamental group of $\mathbb{P}^1\backslash\{0, 1, \infty\}$, the Ihara action and the depth filtration. In § 5 we discuss the linearized double shuffle relations from the Hopf algebra point of view. In § 6, and throughout the rest of the paper, we use polynomial

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representations to replace words of fixed $\mathfrak{D}$-degree r in e_0, e_1 with polynomials in r variables:

$$\bar{\rho} : \mathrm{gr}^{\mathfrak{D}}_r \mathfrak{g} \longrightarrow \mathbb{Q}[x_1, \ldots, x_r],$$

which sends words beginning in e_0 to zero, and $\bar{\rho}(e_1 e_0^{n_1} \ldots e_1 e_0^{n_r}) = x_1^{n_1} \ldots x_r^{n_r}$. This replaces identities between non-commutative formal power series with functional equations in commutative polynomials, strongly reminiscent of those considered in [Eca03, IKZ06]. We show that in the polynomial representation, the Ihara bracket has an extremely simple form (§ 6.5). A simple way to view the duality between depth-graded motivic multiple zeta values and polynomials is via the generating series

$$\sum_{n_1, \ldots, n_r \geq 1} \zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r)\, x_1^{n_1 - 1} \ldots x_r^{n_r - 1}.$$

The generators (1.6) are simply the coefficients of $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n+1)$:

$$\bar{\rho}(\bar{\sigma}_{2n+1}) = x_1^{2n}, \quad \text{for } n \geq 1.$$

In § 7 we review the relation between period polynomials and depth 2 multiple zeta values, and in § 8 we define, for each period polynomial P, an element

$$\bar{\rho}(e_P) \in \mathbb{Q}[x_1, x_2, x_3, x_4],$$

which defines the exceptional elements in $\mathfrak{ls}_4$. These elements satisfy some remarkable properties (§ 9) which are stable under the Ihara bracket. In § 10 we discuss Conjecture 1 and its consequences, and in § 11 we discuss some applications for the enumeration of the totally odd multiple zeta values $\zeta(2n_1 + 1, \ldots, 2n_r + 1)$ where $n_i \geq 1$.

1.5.1 *Related work.* Since the first draft of this paper appeared, there have been a number of related developments, which cannot all be mentioned here for reasons of space. I apologize to the many people who have subsequently extended some of the ideas in this paper in various directions [Mat16, Tas16, Ma16, Li19], not only for the delay in publishing this work, but also for being unable to give a complete survey of subsequent developments of the subject here.

First of all, an alternative description of depth 4 exceptional generators was given in [Bro17a], by constructing canonical zeta elements in $\mathfrak{g}^{\mathfrak{m}}/\mathfrak{D}^4\mathfrak{g}^{\mathfrak{m}}$ and applying the differential in the depth spectral sequence. These elements are motivic (i.e. lie in $\mathfrak{d}\mathfrak{g}^{\mathfrak{m}}_4$), but their relationship to the exceptional elements e defined here is far from clear. The entire construction relies on the relationship between $\mathbb{P}^1 \backslash \{0, 1, \infty\}$ (genus 0) and the unipotent completion of the fundamental group Tate elliptic curve (genus 1), and the fact that the depth filtration is induced by natural filtrations in the elliptic setting. Similarly, the precise relationship between the work of Pollack [Pol09] and the present paper is now partially understood but warrants further investigation.

Subsequently, the work [Bro14b] explains the origin of the quadratic relations between $\bar{\sigma}_{2n+1}$ by proving that they come from 'modular elements' corresponding to non-critical values of L-functions of cusp forms, which act on the relative completion of the fundamental group on the moduli stack $\mathcal{M}_{1,1}$ of elliptic curves. From this perspective, the canonical generators $\bar{\sigma}_{2n+1}$ can be understood as coming from Eisenstein series, which supports the philosophy that Conjecture 2 relates entirely to modular forms. Nevertheless, the connection between modular elements and the phenomena in depth 4 studied in the present paper remain unexplored.

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In a very different direction, Goncharov [Gon05] has studied the depth filtration from the perspective of the homology of the general linear group $\mathrm{GL}_d(\mathbb{Z})$, which he relates to the structure of multiple zeta values in depth d. We have no understanding of the relationship between this point of view and conjecture (1.11).

After the first draft of this paper appeared, Conjecture 4 was related to questions of Koszulity in the paper [EL16].

Finally, the interested reader may wish to consult the notes[5] where, in answer to a question due to Zagier, we reformulated the Broadhurst–Kreimer conjecture as a short exact sequence, which suggests another line of attack on Conjecture 2.

2. Reminders on $\pi_1^{\mathfrak{m}}(\mathbb{P}^1\backslash\{0,1,\infty\})$

2.1 The motivic π_1 of $\mathbb{P}^1\backslash\{0,1,\infty\}$

Let $X = \mathbb{P}^1\backslash\{0,1,\infty\}$, and let $\vec{1}_0, -\vec{1}_1$ denote the tangential base points on X given by the tangent vector 1 at 0, and the tangent vector -1 at 1. Denote the de Rham realization of the motivic fundamental torsor of paths on X with respect to these basepoints by

$$ {}_0\Pi_1 = \pi_1^{\mathrm{dR}}(X, \vec{1}_0, -\vec{1}_1). $$

It is the affine scheme over $\mathbb{Q}$ which to any commutative unitary $\mathbb{Q}$-algebra R associates the set of group-like formal power series in two non-commuting variables e_0 and e_1,

$$ \{S \in R\langle\langle e_0, e_1\rangle\rangle^\times : \Delta S = S\hat{\otimes} S\}, $$

where Δ is the completed coproduct for which the elements e_0 and e_1 are primitive: $\Delta e_i = 1\otimes e_i + e_i \otimes 1$ for $i = 0, 1$. The ring of regular functions on ${}_0\Pi_1$ is the $\mathbb{Q}$-algebra

$$ \mathcal{O}({}_0\Pi_1) \cong \mathbb{Q}\langle e^0, e^1\rangle $$

whose underlying vector space is spanned by the set of words w in the letters e^0, e^1, together with the empty word, and whose multiplication is given by the shuffle product $ш : \mathbb{Q}\langle e^0, e^1\rangle \otimes_{\mathbb{Q}} \mathbb{Q}\langle e^0, e^1\rangle \to \mathbb{Q}\langle e^0, e^1\rangle$. The deconcatenation of words defines a coproduct, making $\mathcal{O}({}_0\Pi_1)$ into a Hopf algebra. This gives rise to a group structure on ${}_0\Pi_1(\mathbb{Q})$ (corresponding to the fact that in the de Rham realization there is a canonical path between any two points on X). Any word w in e^0, e^1 defines a function

$$ {}_0\Pi_1(R) \longrightarrow R $$

which extracts the coefficient S_w of the word w (viewed in e_0, e_1) in a group-like series $S \in R\langle\langle e_0, e_1\rangle\rangle^\times$. The Lie algebra of ${}_0\Pi_1(\mathbb{Q})$ is the completed Lie algebra $\mathbb{L}(e_0, e_1)^\wedge$ of the graded Lie algebra $\mathbb{L}(e_0, e_1)$ which is freely generated by the two elements e_0, e_1 in degree -1. The universal enveloping algebra $\mathcal{U}\,\mathbb{L}(e_0, e_1)$ of $\mathbb{L}(e_0, e_1)$ is the tensor (co)algebra on e_0, e_1:

$$ T(e_0, e_1) = \bigoplus_{n\geq 0} (\mathbb{Q}\, e_0 \oplus \mathbb{Q}\, e_1)^{\otimes n}. \tag{2.1} $$

It is the graded cocommutative Hopf algebra which is the graded dual of $\mathcal{O}({}_0\Pi_1)$. Its multiplication is given by the concatenation product, and its coproduct is the unique coproduct for which e_0 and e_1 are primitive.

[5] www.ihes.fr/brown/BKExactSeq1.pdf.

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2.2 Action of the motivic Galois group

Now let $\mathcal{MT}(\mathbb{Z})$ denote the Tannakian category of mixed Tate motives over $\mathbb{Z}$, with canonical fiber functor given by the de Rham realization. Let $\mathcal{G}_{\mathcal{MT}(\mathbb{Z})}$ denote the group of automorphisms of this fiber functor. It is an affine group scheme over $\mathbb{Q}$. It has a decomposition as a semi-direct product

$$\mathcal{G}_{\mathcal{MT}(\mathbb{Z})} \cong \mathcal{U}_{\mathcal{MT}(\mathbb{Z})} \rtimes \mathbb{G}_m,$$

where $\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$ is pro-unipotent. Furthermore, one knows from the relationship between the Ext groups in $\mathcal{MT}(\mathbb{Z})$ and Borel's results on the rational algebraic K-theory of $\mathbb{Q}$ that the graded Lie algebra of $\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$ is non-canonically isomorphic to the Lie algebra freely generated by one generator σ_{2i+1} in degree $-(2i+1)$ for every $i \geq 1$. It is important to note that only the classes of the elements σ_{2i+1} in the abelianization $\mathcal{U}^{\mathrm{ab}}_{\mathcal{MT}(\mathbb{Z})}$ are canonical, the elements σ_{2i+1} themselves are not.

Since $\mathcal{O}({}_0\Pi_1)$ is the de Rham realization of an Ind-object in the category $\mathcal{MT}(\mathbb{Z})$, there is an action of the motivic Galois group $\mathcal{G}_{\mathcal{MT}(\mathbb{Z})}$ on ${}_0\Pi_1$ and hence

$$\mathcal{U}_{\mathcal{MT}(\mathbb{Z})} \times {}_0\Pi_1 \longrightarrow {}_0\Pi_1. \tag{2.2}$$

The action of $\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$ on the unit element $1 \in {}_0\Pi_1$ defines a map

$$g \mapsto g(1) : \mathcal{U}_{\mathcal{MT}(\mathbb{Z})} \longrightarrow {}_0\Pi_1, \tag{2.3}$$

and the action (2.2) factors through a map

$$\circ : {}_0\Pi_1 \times {}_0\Pi_1 \longrightarrow {}_0\Pi_1 \tag{2.4}$$

first computed by Ihara. It is obtained from [DG05, §§ 5.9, 5.13], by reversing all words in order to be consistent with our convention for composition of paths. An element $a \in {}_0\Pi_1$ defines an action denoted by $\langle a\rangle_0$ on ${}_0\Pi_0$ which is compatible with (2.4) via the composition of paths ${}_0\Pi_0 \times {}_0\Pi_1 \to {}_0\Pi_1$. Therefore, writing x_{00} (respectively, x_{01}) for the element x in ${}_0\Pi_0$ (respectively, ${}_0\Pi_1$), one finds that for $g \in {}_0\Pi_1$,

$$a \circ g = a \circ g_{01} = a \circ (g_{00}.1_{01}) = \langle a\rangle_0(g).a(1_{01}) = (\langle a\rangle_0(g)).a, \tag{2.5}$$

where $\langle a\rangle_0$ acts on the generators $\exp(e_i)$ in ${}_0\Pi_0$, for $i = 0, 1$, by

$$\begin{aligned} \langle a\rangle_0(\exp(e_0)) &= \exp(e_0), \\ \langle a\rangle_0(\exp(e_1)) &= a\exp(e_1)a^{-1}. \end{aligned} \tag{2.6}$$

We now give a concrete way to compute $\circ$ by expressing it as the restriction of a combinatorially defined map $\underline{\circ}$ on a larger space.

DEFINITION 2.1. Inductively define a $\mathbb{Q}$-bilinear map

$$\underline{\circ} : T(e_0, e_1) \otimes T(e_0, e_1) \longrightarrow T(e_0, e_1)$$

as follows. For any two words a, w in e_0, e_1, and any integer $n \geq 0$, let

$$a \,\underline{\circ}\, (e_0^n e_1 w) = e_0^n a e_1 w + e_0^n e_1 a^* w + e_0^n e_1 (a \,\underline{\circ}\, w), \tag{2.7}$$

where $a \,\underline{\circ}\, e_0^n = e_0^n a$, and for any $a_i \in \{e_0, e_1\}$, $(a_1 \dots a_n)^* = (-1)^n a_n \dots a_1$.

We now show that the map $\underline{\circ}$ restricts to the full action

$$\mathfrak{g} \otimes_{\mathbb{Q}} \mathcal{U}\,\mathrm{Lie}\,{}_0\Pi_1 \to \mathcal{U}\,\mathrm{Lie}\,{}_0\Pi_1 \tag{2.8}$$

induced by (2.4). To see this, identify the universal enveloping of the graded Lie algebra $\mathcal{U}\,\mathrm{Lie}\,{}_0\Pi_1 = \mathcal{U}\mathbb{L}(e_0, e_1)$ with $T(e_0, e_1)$. Since $\mathfrak{g}$ is isomorphic (as a vector space) to $\mathbb{L}(e_0, e_1)$, there is also a natural embedding $i : \mathfrak{g} \to T(e_0, e_1)$.

Proposition 2.2. *The action* (2.8) *is obtained by restriction of* $\underline{\circ}$, *that is,*

$$a \circ b = i(a)\,\underline{\circ}\,b.$$

Proof. For any $S \in {}_0\Pi_1$, the coefficient of w in S^{-1} is equal to the coefficient of w^* in S, since the map $*$ is the antipode in $\mathcal{O}({}_0\Pi_1)$. Identifying the (vector space) $\mathfrak{g} \cong \mathbb{L}(e_0, e_1)$ with its image in $T(e_0, e_1)$, it follows that the infinitesimal, weight-graded, version of the map (2.6) is the derivation $\langle f\rangle_0 : \mathbb{L}(e_0, e_1) \to \mathbb{L}(e_0, e_1)$ which for any $f \in \mathbb{L}(e_0, e_1)$ is given by

$$e_0 \mapsto 0, \quad e_1 \mapsto f e_1 + e_1 f^*.$$

Thus $\langle f\rangle_0 : T(e_0, e_1) \to T(e_0, e_1)$ is the map

$$\begin{aligned}\langle f\rangle_0\,(e_0^{m_0} e_1 \dots e_1 e_0^{m_r}) = e_0^{m_0}&(f e_1 + e_1 f^*) e_0^{m_1} e_1 \cdots e_0^{m_{r-1}} e_1 e_0^{m_r}\\ &+ \cdots + e_0^{m_0} e_1 e_0^{m_1} \cdots e_0^{m_{r-1}} (f e_1 + e_1 f^*) e_0^{m_r}.\end{aligned}$$

Adding the term $e_0^{m_0} e_1 \dots e_1 e_0^{m_r} f$ corresponding to concatenation on the right by f gives precisely the map defined by (2.7). □

2.3 The motivic Lie algebra

By (2.3), we obtain a map of Lie algebras

$$\mathrm{Lie}(\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}) \longrightarrow \mathfrak{g} = \big(\mathbb{L}(e_0, e_1)\ ,\ \{\,,\}\big), \tag{2.9}$$

where the Ihara bracket satisfies $\{f, g\} = f \circ g - g \circ f$. It follows from Theorem 1.1 that this map is injective [Bro12]. In this paper, we shall identify $\mathrm{Lie}(\mathcal{U}_{\mathcal{MT}(\mathbb{Z})})$ with its image, and abusively call it the motivic Lie algebra.

Definition 2.3. The motivic Lie algebra $\mathfrak{g}^{\mathfrak{m}} \subseteq \mathfrak{g}$ is the image of the map (2.9).

The Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ is non-canonically isomorphic to the free Lie algebra with one generator σ_{2i+1} in each degree $-(2i + 1)$ for $i \geq 1$.

3. Motivic multiple zeta values

Let $\mathcal{A}^{\mathcal{MT}}$ denote the graded Hopf algebra of functions on $\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$. Dualizing (2.2) gives the motivic coaction (written in this paper as a left coaction)

$$\Delta^{\mathcal{M}} : \mathcal{O}({}_0\Pi_1) \longrightarrow \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1).$$

Furthermore, the image in ${}_0\Pi_1(\mathbb{C})$ of the straight path dch from 0 to 1 in X under the comparison isomorphism is the Drinfeld associator element $\Phi \in {}_0\Pi_1(\mathbb{R})$ which begins

$$\Phi = 1 + \zeta(2)[e_1, e_0] + \zeta(3)([e_1, [e_1, e_0]] + [e_0, [e_0, e_1]]) + \cdots .$$

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The map which takes the coefficient of a word w in Φ defines the period homomorphism

$$per : \mathcal{O}({}_0\Pi_1) \longrightarrow \mathbb{R}.$$

Here, we use the convention from [Bro12]: the coefficient of the word $e_{a_1} \dots e_{a_n}$ in Φ, for $a_i \in \{0,1\}$, is the iterated integral

$$\int_0^1 \omega_{a_1} \dots \omega_{a_n}$$

regularized with respect to the tangent vector 1 at 0, and -1 at 1, where the integration begins on the left, and $\omega_0 = dt/t$ and $\omega_1 = dt/(1-t)$.

Definition 3.1. The algebra of motivic multiple zeta values is defined as follows. The ideal of motivic relations between multiple zeta values is defined to be $J^{\mathcal{MT}} \leq \mathcal{O}({}_0\Pi_1)$, the largest graded ideal contained in the kernel of per which is stable under $\Delta^{\mathcal{M}}$. We set

$$\mathcal{H} = \mathcal{O}({}_0\Pi_1)/J^{\mathcal{MT}},$$

and let $\zeta^{\mathfrak{m}}(n_1, \dots, n_r)$ denote the image of the word $e^1(e^0)^{n_1-1} \dots e^1(e^0)^{n_r-1}$ in $\mathcal{H}$. Likewise, for any $a_1, \dots, a_n \in \{0,1\}$, we let $I^{\mathfrak{m}}(0; a_1, \dots, a_n; 1)$ denote the image of the word $e^{a_1} \dots e^{a_n}$ in $\mathcal{H}$. Equivalently, one can define

$$I^{\mathfrak{m}}(0; a_1, \dots, a_n; 1) = [\mathcal{O}(\pi_1^{\mathrm{mot}}(X, \vec{1}_0, -\vec{1}_1), dch, e^{a_1} \dots e^{a_n}]^{\mathfrak{m}},$$

where the right-hand side is a motivic period [Bro14a] of the category $\mathcal{MT}(\mathbb{Z})$, and define the motivic multiple zeta values by specializing to the case when $a_1 = 1$ and $a_n = 0$.

Remark 3.2. The algebra of motivic multiple zeta values has the following geometric interpretation: $J^{\mathcal{MT}}$ is the ideal of functions which vanishes on the orbit of the de Rham image of dch in ${}_0\Pi_1(\mathbb{C})$. The latter is defined over $\mathbb{Q}$ because it is the image under the comparison isomorphism of the orbit under the Betti Galois group $\mathrm{Aut}^{\otimes}_{\mathcal{MT}(\mathbb{Z})}(\omega_B)$ of the Betti image of the straight-line path, which is rational.

The space $\mathcal{H}$ is naturally graded by the weight, and has a graded coaction

$$\Delta^{\mathcal{M}} : \mathcal{H} \longrightarrow \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathcal{H} \tag{3.1}$$

and a period map $per : \mathcal{H} \to \mathbb{R}$. The period of $\zeta^{\mathfrak{m}}(n_1, \dots, n_r)$ is $\zeta(n_1, \dots, n_r)$. One obtains partial information about the motivic coaction (3.1) using the fact that it factors through the coaction which is dual to the Ihara action (2.4).

3.1 The Ihara coaction

For any graded Hopf algebra H, let $IH = H_{>0}/H_{>0}^2$ denote the Lie coalgebra of indecomposable elements of H, and let $\pi : H_{>0} \to IH$ denote the natural map. Dualizing (2.8) (and making it into a left coaction) gives an infinitesimal coaction

$$\mathcal{O}({}_0\Pi_1) \longrightarrow I\mathcal{O}({}_0\Pi_1) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1). \tag{3.2}$$

Let $D_r : \mathcal{O}({}_0\Pi_1) \to I\mathcal{O}({}_0\Pi_1)_r \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1)$ denote its component of degree $(r, \cdot)$, and let us denote the element $e^{a_1} \dots e^{a_n}$ in $\mathcal{O}({}_0\Pi_1)$ by $\mathbb{I}(0; a_1, \dots, a_n; 1)$, where $a_i \in \{0,1\}$.

Proposition 3.3. *Set $a_0 = 0, a_{n+1} = 1$. For all $r \geq 1$, and $a_1, \ldots, a_n \in \{0,1\}$,*

$$D_r \, \mathbb{I}(0; a_1, \ldots, a_n; 1) = \sum_{p=0}^{n-r} \pi(\mathbb{I}(a_p; a_{p+1}, \ldots, a_{p+r}; a_{p+r+1})) \otimes \mathbb{I}(0; a_1, \ldots, a_p, a_{p+r+1}, \ldots, a_n; 1), \tag{3.3}$$

where $\mathbb{I}(a_p; a_{p+1}, \ldots, a_{p+r}; a_{p+r+1}) \in \mathcal{O}({}_0\Pi_1)$ is defined to be zero if $a_p = a_{p+r+1}$, and equal to $(-1)^r \mathbb{I}(a_{p+r+1}; a_{p+r}, \ldots, a_{p+1}; a_p)$ if $a_p = 1$ and $a_{p+r+1} = 0$.

Proof. One checks that this formula is dual to $\underline{\circ}$ (see also [Bro14a, § 2.5]). □

Since the motivic coaction on $\mathcal{H}$ factors through the Ihara coaction, it follows that the degree $(r, \cdot)$ component factors through operators

$$D_r : \mathcal{H} \longrightarrow I\mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$$

given by the same formula as (3.3) in which each term $\mathbb{I}$ is replaced by its image $I^{\mathfrak{m}}$ in $\mathcal{H}$ (respectively, $\mathcal{A}$). Since $\mathcal{A}^{\mathcal{MT}}$ is cogenerated in odd degrees only, the motivic coaction on $\mathcal{H}$ is completely determined by the set of operators D_{2r+1} for all $r \geq 1$ (see [Bro12]).

4. The depth filtration

4.1 Definition

The depth filtration was defined in [DG05, § 6.1]. We recall the definition in a slightly different language. The inclusion $\mathbb{P}^1 \backslash \{0, 1, \infty\} \hookrightarrow \mathbb{P}^1 \backslash \{0, \infty\}$ induces a map on the motivic fundamental groupoids

$$\pi_1^{\mathrm{mot}}(X, \vec{1}_0, -\vec{1}_1) \to \pi_1^{\mathrm{mot}}(\mathbb{G}_m, \vec{1}_0, 1), \tag{4.1}$$

and hence on the de Rham realizations

$$\mathcal{O}(\pi_1^{\mathrm{dR}}(\mathbb{G}_m, \vec{1}_0, 1)) \longrightarrow \mathcal{O}({}_0\Pi_1),$$

and similarly for $\mathcal{O}(\pi_1^{\mathrm{dR}}(\mathbb{G}_m, \vec{1}_0)) \to \mathcal{O}({}_0\Pi_0)$. They are given by the inclusion of $\mathbb{Q}\langle e^0 \rangle$ into $\mathbb{Q}\langle e^0, e^1 \rangle$. Define their images to be $\mathfrak{D}_0 \mathcal{O}({}_0\Pi_1)$ and $\mathfrak{D}_0 \mathcal{O}({}_0\Pi_0)$, respectively. Now define increasing filtrations $\mathfrak{D}_d$ on $\mathcal{O}({}_0\Pi_0)$ and $\mathcal{O}({}_0\Pi_1)$ by induction on $d \geq 0$ as follows: $\mathfrak{D}_d$ is the largest subspace such that $\Delta \mathfrak{D}_d \subset \sum_{i+j=d} \mathfrak{D}_i \otimes \mathfrak{D}_j$, where $\Delta^{\mathrm{dec}} : \mathcal{O}({}_0\Pi_x) \to \mathcal{O}({}_0\Pi_x) \otimes \mathcal{O}({}_0\Pi_0)$ is dual to composition of paths, for $x = 0, 1$. Since Δ^{dec}, on identifying $\mathcal{O}({}_0\Pi_0) \cong \mathcal{O}({}_0\Pi_1) \cong \mathbb{Q}\langle e_0, e_1 \rangle$, is nothing other than the deconcatenation coproduct, the filtration $\mathfrak{D}_d \mathcal{O}({}_0\Pi_1)$ is given by

$$\mathfrak{D}_d \mathcal{O}({}_0\Pi_1) = \langle \text{words } w \text{ such that } \deg_{e^1} w \leq d \rangle_{\mathbb{Q}}, \tag{4.2}$$

with respect to which $\mathcal{O}({}_0\Pi_1)$ is a filtered comodule over the filtered Hopf algebra $\mathcal{O}({}_0\Pi_0)$, with respect to Δ^{dec}. Furthermore, since the map (4.1) is motivic, it follows that $\mathfrak{D}_0$ is preserved by the action of the motivic Galois group. The same is true for all d by induction: if $g \in G^{\mathrm{dR}}_{\mathcal{MT}(\mathbb{Z})}$ and $g \, \mathfrak{D}_i \subset \mathfrak{D}_i$ for all $i < d$, then we also have $g \mathfrak{D}_d \subset \mathfrak{D}_d$ by definition of $\mathfrak{D}_d$, since g commutes with Δ^{dec}, which is motivic. Therefore the depth is also motivic and descends to the algebra $\mathcal{H}$.

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By Definition 3.1 the depth filtration $\mathfrak{D}_d\mathcal{H}$ is the increasing filtration defined by

$$\mathfrak{D}_d\mathcal{H} = \langle \zeta^{\mathfrak{m}}(n_1, \ldots, n_i) : i \leq d\rangle_{\mathbb{Q}}.$$

Following [Del10], it is convenient to define the $\mathfrak{D}$-degree on $\mathcal{O}({}_0\Pi_1)$ to be the degree in e^1. It defines a grading on ${}_0\Pi_1$ which is not motivic. By (4.2), the depth filtration (which is motivic) is simply the increasing filtration associated to the $\mathfrak{D}$-degree.

4.2 Depth-graded motivic multiple zeta values

Definition 4.1. Let $\mathfrak{D}_d\mathcal{A}$ be the induced filtration on the quotient $\mathcal{A} = \mathcal{H}/\zeta^{\mathfrak{m}}(2)\mathcal{H}$. We define the *depth-graded motivic multiple zeta value*

$$\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r)$$

to be the image of $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$ in $\mathrm{gr}^{\mathfrak{D}}_r\mathcal{H}$.

Proposition 4.2. *There is a non-canonical isomorphism of bigraded vector spaces:*

$$\mathrm{gr}^{\mathfrak{D}}\mathcal{H} \cong \mathrm{gr}^{\mathfrak{D}}\mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2)], \tag{4.3}$$

where $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2)^n$ are in depth 1 for all $n \geq 1$.

Proof. Choose a homomorphism $\pi_2 : \mathcal{H} \to \mathbb{Q}[\zeta^{\mathfrak{m}}(2)]$ which respects the weight-grading and such that $\pi_2(\zeta^{\mathfrak{m}}(2)) = \zeta^{\mathfrak{m}}(2)$. Such a homomorphism exists by [DG05, § 5.20] (see [Bro12, § 2.3]). Composing with the coaction (3.1), we obtain a map

$$\mathcal{H} \xrightarrow{\Delta^{\mathcal{M}}} \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H} \xrightarrow{id\otimes\pi_2} \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)].$$

By a motivic version [Bro12] of Euler's theorem, $\zeta^{\mathfrak{m}}(2)^n$ is a rational multiple of $\zeta^{\mathfrak{m}}(2n)$, and so all powers of $\zeta^{\mathfrak{m}}(2)$ have depth 1. The depth filtration thus satisfies

$$\mathbb{Q} = \mathfrak{D}_0\mathbb{Q}[\zeta^{\mathfrak{m}}(2)] \subset \mathfrak{D}_1\mathbb{Q}[\zeta^{\mathfrak{m}}(2)] = \mathbb{Q}[\zeta^{\mathfrak{m}}(2)].$$

Since $\mathfrak{D}_0\mathcal{H} = \mathbb{Q}$, it follows trivially that π_2 respects the depth filtration because it is $\mathbb{Q}$-linear. Since the depth filtration is motivic, it is also respected by $\Delta^{\mathcal{M}}$, and therefore the map $(id \otimes \pi_2)\,\Delta^{\mathcal{M}} : \mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)]$ defined above also respects the depth filtration. The statement (4.3) follows since we know that this map is an isomorphism (by [Bro12, (2.13)] or [Del10, Proposition 5.8]). □

Since $\mathrm{gr}^{\mathfrak{D}}\mathcal{A}$ is a commutative graded Hopf algebra (for the coproduct induced by $\Delta^{\mathcal{M}}$), it is a polynomial algebra. The same is then true for $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}$, by (4.3). If I denotes indecomposable elements, then it follows that $I(\mathrm{gr}^{\mathfrak{D}}\mathcal{A}) \cong \mathrm{gr}^{\mathfrak{D}}\, I\mathcal{A}$.

4.3 Depth-graded motivic Lie algebra

The depth filtration defines a decreasing filtration $\mathfrak{D}^r$ on $\mathfrak{g}^{\mathfrak{m}}$ where $\mathfrak{D}^r$ consists of words with at least r occurrences of e_1:

$$\mathfrak{D}^r\mathfrak{g}^{\mathfrak{m}} = \langle w \in \mathfrak{g}^{\mathfrak{m}} : \deg_{e_1} w \geq r\rangle.$$

We denote the associated graded Lie algebra by $\mathfrak{dg}^{\mathfrak{m}}$. There is correspondingly a decreasing depth filtration on $\mathcal{U}\mathfrak{g}^{\mathfrak{m}}$, also denoted by $\mathfrak{D}$.

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It follows from the definitions above that $\mathfrak{dg}^{\mathfrak{m}}$ is the bigraded Lie algebra dual to the bigraded coalgebra $I(\mathrm{gr}^{\mathfrak{D}}\mathcal{A}) \cong \mathrm{gr}^{\mathfrak{D}} I\mathcal{A}$ of depth-graded motivic multiple zeta values modulo products. Thus the problem of studying relations between (motivic) multiple zeta values modulo lower depth (and modulo $\zeta^{\mathfrak{m}}(2)$) and the algebra $\mathfrak{dg}^{\mathfrak{m}}$ are equivalent.

4.4 Depth-parity

The following proposition is a consequence of Tsumura's result on double shuffle equations (Proposition 6.4).

Proposition 4.3. *The depth-graded motivic Lie algebra $\mathfrak{dg}^{\mathfrak{m}}$ vanishes in bidegrees with different parity. More precisely, it vanishes in weight N and depth r if $N \not\equiv r \pmod 2$.*

Equivalently, if $n_1 + \cdots + n_r \not\equiv r \pmod 2$, and $n_1 + \cdots + n_r > 2$ then

$$\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r) \equiv 0 \quad (\text{mod products}). \tag{4.4}$$

We do not need to work modulo $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2)$ in the previous equation since the weight is larger than 2 by assumption and all other even zeta values $\zeta^{\mathfrak{m}}(2n)$, $n \geq 2$, are products.

4.5 Depth spectral sequence

The depth filtration on the motivic Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ induces a homology spectral sequence which converges to the associated graded for the depth of the homology of $\mathfrak{g}^{\mathfrak{m}}$. By Theorem 1.1, the latter satisfies

$$H_i(\mathfrak{g}^{\mathfrak{m}}) = \begin{cases} \bigoplus_{n\geq 1} \mathbb{Q}[\sigma_{2n+1}] & \text{if } i = 1 \\ 0 & \text{if } i \geq 1 \end{cases}$$

and is entirely concentrated in depth 1.

The depth spectral sequence satisfies

$$E^1_{-p,q} = \mathrm{gr}^p_{\mathfrak{D}} H_{q-p}(\mathfrak{dg}^{\mathfrak{m}}),$$

where $E^1_{-p,q}$ vanishes unless $p \geq 1$ and $p < q \leq 2p$, as can easily be seen from the Chevalley–Eilenberg chain complex which computes the homology of a Lie algebra (see § 10.2 and (10.3)). The differentials satisfy

$$d^r_{p,q} : E^r_{p,q} \to E^r_{p-r,q+r-1}.$$

Proposition 4.4. *The differentials d^r vanish if r is odd.*

Proof. The weight grading on $\mathfrak{dg}^{\mathfrak{m}}$ induces a weight grading on the depth spectral sequence, with respect to which the differentials are of degree 0. It follows from Proposition 4.3 and $E^1_{-p,q} = \mathrm{gr}^p_{\mathfrak{D}} H_{q-p}(\mathfrak{dg}^{\mathfrak{m}})$ that $E^1_{p,q}$, and hence all $E^r_{p,q}$, vanish unless the depth and weight have the same parity. The result follows since d^r has (weight, depth)-bidegree $(0, r)$. $\square$

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Here is a picture of the potentially non-vanishing $E^1 = E^2$ terms:

$$
\begin{array}{ccccc|c}
\ddots & \mathrm{gr}^4_{\mathfrak{D}} H_4 & & & & 8 \\
 & \mathrm{gr}^4_{\mathfrak{D}} H_3 & & & & 7 \\
 & \mathrm{gr}^4_{\mathfrak{D}} H_2 & \mathrm{gr}^3_{\mathfrak{D}} H_3 & & & 6 \\
 & \mathrm{gr}^4_{\mathfrak{D}} H_1 & \mathrm{gr}^3_{\mathfrak{D}} H_2 & & & 5 \\
 & & \mathrm{gr}^3_{\mathfrak{D}} H_1 & \mathrm{gr}^2_{\mathfrak{D}} H_2 & & 4 \\
 & & & \mathrm{gr}^2_{\mathfrak{D}} H_1 & & 3 \\
 & & & & \mathrm{gr}^1_{\mathfrak{D}} H_1 & 2 \\
 & & & & & 1 \\
\hline
\dots & -4 & -3 & -2 & -1 &
\end{array}
$$

In fact, we know by Theorem 1.1 that

$$\mathrm{gr}^1_{\mathfrak{D}} H_1(\mathfrak{d}\mathfrak{g}^{\mathfrak{m}}) \cong H_1(\mathfrak{g}^{\mathfrak{m}}) \cong \bigoplus_{n \geq 1} \mathbb{Q}[\sigma_{2n+1}],$$

and therefore everything to the left of the column indexed -1 converges to zero. Furthermore, one knows that $\mathrm{gr}^2_{\mathfrak{D}} H_1(\mathfrak{d}\mathfrak{g}^{\mathfrak{m}}) = 0$, and $\mathrm{gr}^3_{\mathfrak{D}} H_i(\mathfrak{d}\mathfrak{g}^{\mathfrak{m}})$ vanish for all i. One also has a complete description of $\mathrm{gr}^2_{\mathfrak{D}} H_2(\mathfrak{d}\mathfrak{g}^{\mathfrak{m}})$ in terms of period polynomials of cusp forms, as discussed below. Therefore, the first interesting part of the differential is

$$d^2 : \mathrm{gr}^2_{\mathfrak{D}} H_2(\mathfrak{d}\mathfrak{g}^{\mathfrak{m}}) \longrightarrow \mathrm{gr}^4_{\mathfrak{D}} H_1(\mathfrak{d}\mathfrak{g}^{\mathfrak{m}}),$$

and the main Conjecture 1 can be reformulated as saying that the components of all other differentials in the depth spectral sequence vanish.

5. Linearized double shuffle relations

5.1 Reminders on the standard relations

We briefly review the double shuffle relations and their depth-linearized versions. See [Car02, Rac02, Bro17b] for further background.

5.1.1 *Shuffle product.* Consider the algebra $\mathbb{Q}\langle e_0, e_1\rangle$ of words in the two letters e_0, e_1, equipped with the shuffle product $\sqcup\!\sqcup$ (§ 2.1). It is defined recursively by

$$e_i w \sqcup\!\sqcup e_j w' = e_i(w \sqcup\!\sqcup e_j w') + e_j(e_i w \sqcup\!\sqcup w') \tag{5.1}$$

for all $w, w' \in \{e_0, e_1\}^{\times}$ and $i, j \in \{0, 1\}$, and the property that the empty word 1 satisfies $1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w$. It is a Hopf algebra for the deconcatenation coproduct. A linear map $\Phi : \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}$ is a homomorphism for the shuffle multiplication, or $\Phi_w \Phi_{w'} = \Phi_{w \sqcup\!\sqcup w'}$ for all $w, w' \in \{e_0, e_1\}^{\times}$ and $\Phi_1 = 1$, if and only if the series

$$\Phi = \sum_w \Phi_w w \in \mathbb{Q}\langle\langle e_0, e_1\rangle\rangle$$

is invertible and group-like for the (completed) coproduct $\Delta_{\sqcup\!\sqcup}$ with respect to which e_0 and e_1 are primitive (compare § 2.1). In other words, there is an equivalence:

$$\Phi \text{ homomorphism for } \sqcup\!\sqcup \quad \Longleftrightarrow \quad \Phi \in \mathbb{Q}\langle\langle e_0, e_1\rangle\rangle^{\times} \text{ and } \Delta_{\sqcup\!\sqcup}\Phi = \Phi \hat{\otimes} \Phi. \tag{5.2}$$

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One says that Φ satisfies the shuffle relations if either of the equivalent conditions (5.2) holds. Passing to the corresponding Lie algebra, we have an equivalence

$$\Phi_{w \,ш\, w'} = 0 \text{ for all } w, w' \quad \Longleftrightarrow \quad \Phi \in \mathbb{Q}\langle\langle e_0, e_1\rangle\rangle \text{ and } \Delta_ш \Phi = 1\hat{\otimes}\Phi + \Phi\hat{\otimes}1. \tag{5.3}$$

One says that Φ satisfies the shuffle relations *modulo products* if either of the equivalent conditions (5.3) holds.

The algebra $\mathbb{Q}\langle e_0, e_1\rangle$ is bigraded for the degree, or weight (for which e_0, e_1 both have degree -1), and the $\mathfrak{D}$-degree for which e_1 has degree 1, and e_0 degree 0. The relations (5.1)–(5.3) evidently respect both gradings. In this case, then, passing to the depth grading does not change the relations in any way, and the linearized shuffle relations are identical to the shuffle relations modulo products.

Definition 5.1. Let $\Phi \in \mathrm{gr}^r_{\mathfrak{D}} T(e_0, e_1)$ be of weight N. It defines a linear form $w \mapsto \Phi_w$ on words of weight $N \geq 2$ and $\mathfrak{D}$-degree r. It satisfies the *linearized shuffle relations* if

$$\Delta'_ш \Phi = 0,$$

where $\Delta'_ш$ is the reduced coproduct $\Delta'_ш(\Phi) = \Delta_ш(\Phi) - 1 \otimes \Phi - \Phi \otimes 1$. Equivalently, $\Phi_{w \,ш\, w'} = 0$ for all words $w, w' \in \{e_0, e_1\}^\times$ of total weight N and total $\mathfrak{D}$-degree r.

5.1.2 *Stuffle product.* Let $Y = \{\mathsf{y}_n, n \geq 1\}$ denote an alphabet with one letter y_i in every degree ≥ 1, and consider the graded algebra $\mathbb{Q}\langle Y\rangle$ equipped with the stuffle product [Rac02]. It is defined recursively by

$$\mathsf{y}_i w * \mathsf{y}_j w' = \mathsf{y}_i(w * \mathsf{y}_j w') + \mathsf{y}_j(\mathsf{y}_i w * w') + \mathsf{y}_{i+j}(w * w') \tag{5.4}$$

for all $w, w' \in Y^\times$ and $i, j \geq 1$, and the property that the empty word 1 satisfies $1 * w = w * 1 = w$. A linear map $\Phi : \mathbb{Q}\langle Y\rangle \to \mathbb{Q}$ is a homomorphism for the stuffle multiplication, or $\Phi_w \Phi_{w'} = \Phi_{w*w'}$ for all $w, w' \in Y^\times$ and $\Phi_1 = 1$, if and only if

$$\Phi = \sum_w \Phi_w w \in \mathbb{Q}\langle\langle Y\rangle\rangle^\times$$

is group-like for the (completed) coproduct $\Delta_* : \mathbb{Q}\langle\langle Y\rangle\rangle \to \mathbb{Q}\langle\langle Y\rangle\rangle \hat{\otimes}_{\mathbb{Q}} \mathbb{Q}\langle\langle Y\rangle\rangle$ which is a homomorphism for the concatenation product and defined on generators by

$$\Delta_* \mathsf{y}_n = \sum_{i=0}^{n} \mathsf{y}_i \otimes \mathsf{y}_{n-i}. \tag{5.5}$$

Thus the stuffle relations are equivalent to being group-like for Δ_*:

$$\Phi \text{ homomorphism for } * \quad \Longleftrightarrow \quad \Phi \in \mathbb{Q}\langle\langle Y\rangle\rangle^\times \text{ and } \Delta_*\Phi = \Phi\hat{\otimes}\Phi. \tag{5.6}$$

One says that Φ satisfies the stuffle relations if either of the equivalent conditions (5.6) holds. Passing to the corresponding Lie algebra, we have an equivalence

$$\Phi_{w*w'} = 0 \text{ for all } w, w' \quad \Longleftrightarrow \quad \Phi \in \mathbb{Q}\langle\langle Y\rangle\rangle \text{ and } \Delta_*\Phi = 1\hat{\otimes}\Phi + \Phi\hat{\otimes}1. \tag{5.7}$$

One says that Φ satisfies the stuffle relations *modulo products* if either of the equivalent conditions (5.7) holds.

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The algebra $\mathbb{Q}\langle Y\rangle$ is graded for the degree (where y_n has degree n), and filtered for the depth (where y_n has depth 1). By inspection of (5.4), we notice that the rightmost term is of lower depth than the other terms and therefore drops out in the associated graded. The associated graded of $*$ therefore satisfies the same recursive definition as for $ш$ and it follows that the associated depth-graded

$$\mathrm{gr}_{\mathfrak{D}}(\mathbb{Q}\langle Y\rangle, *) \cong (\mathbb{Q}\langle Y\rangle, ш) \tag{5.8}$$

is simply the shuffle algebra on Y. The depth induces a decreasing filtration on the (dual) completed Hopf algebra $\mathbb{Q}\langle\langle Y\rangle\rangle$, and it follows from (5.5) that the images of the elements y_n are primitive in the associated graded. Thus

$$\mathrm{gr}_{\mathfrak{D}}\Delta_* = \Delta_{ш,Y}, \tag{5.9}$$

where $\Delta_{ш,Y} : \mathbb{Q}\langle\langle Y\rangle\rangle \to \mathbb{Q}\langle\langle Y\rangle\rangle\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}\langle\langle Y\rangle\rangle$ is the (completed) coproduct for which the elements y_n are primitive, and which is a homomorphism for concatenation.

Definition 5.2. Let $\Phi \in T(Y)$, the tensor (co)algebra on Y, of degree $N \geq 2$ and $\mathfrak{D}$-degree r. It defines a linear map $w \mapsto \Phi_w$ on words in Y of weight N and $\mathfrak{D}$-degree r. We say that it satisfies the *linearized stuffle relations* if

$$\Delta'_{ш,Y}\Phi = 0,$$

where $\Delta'_{ш,Y} = \Delta_{ш,Y} - 1\otimes \mathrm{id} - \mathrm{id}\otimes 1$ is the reduced coproduct of $\Delta_{ш,Y}$ for which the y_n are primitive. Equivalently, $\Phi_{w\,ш\,w'} = 0$ for all words $w, w' \in Y$ of total weight N and total $\mathfrak{D}$-degree r.

5.1.3 *Linearized double shuffle relations.* In order to consider both relations simultaneously, define a linear map

$$\alpha : \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle Y\rangle$$

which maps every word beginning in e_0 to 0, and such that

$$\alpha(e_1 e_0^{a_1}\dots e_1 e_0^{a_r}) = \mathsf{y}_{a_1+1}\dots \mathsf{y}_{a_r+1}.$$

In [Rac02], Racinet considered a certain graded vector space, denoted $\mathfrak{dm}_0(\mathbb{Q})$ [Rac02, Définition 2.4], of series satisfying the shuffle and stuffle relations and a regularization condition, and showed that it is a Lie algebra for the Ihara bracket. Since we consider the depth-graded version of this algebra, the regularization plays no role here.

Definition 5.3. Let $\Phi \in \mathrm{gr}^{\mathfrak{D}}_r T(e_0, e_1)$ of weight N. The linear form $w \mapsto \Phi_w$ on words of weight N and $\mathfrak{D}$-degree r satisfies the *linearized double shuffle relations* if

$$\Delta'_{ш}\Phi = 0 \quad \text{and} \quad \Delta'_{ш,Y}\,\alpha(\Phi) = 0.$$

When $r = 1$, we add the extra condition that $\Phi = 0$ when N is even, and $\Phi(e_0) = \Phi(e_1) = 0$. Let $\mathfrak{ls} \subset \mathcal{U}\mathfrak{g}$ denote the vector space of elements satisfying the linearized double shuffle relations. It is bigraded by weight and depth.

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Remark 5.4. There is a natural inclusion

$$\mathrm{gr}_{\mathfrak{D}}\mathfrak{dm}_0(\mathbb{Q}) \longrightarrow \mathfrak{ls}. \tag{5.10}$$

The graded subspace of $\mathfrak{ls}$ of weight N and depth d is isomorphic to the vector space denoted $D_{N+d,d}$ in [IKZ06]. In [IKZ06] it is conjectured that (5.10) is an isomorphism.

Racinet proved that $\mathfrak{dm}_0(\mathbb{Q})$ is preserved by the Ihara bracket. Since the latter is homogeneous for the $\mathfrak{D}$-degree, it follows that $\mathrm{gr}_{\mathfrak{D}}\mathfrak{dm}_0(\mathbb{Q})$ is also preserved by the bracket, but this is not quite enough to prove that $\mathfrak{ls}$ is too.

Theorem 5.5. *The bigraded vector space* $\mathfrak{ls}$ *is preserved by the Ihara bracket.*

Proof. The compatibility of the shuffle product with the Ihara bracket follows by definition. It therefore suffices to check that the linearized stuffle relation is preserved by the bracket. The proof of [Rac02] goes through identically, and uses in an essential way the fact that the images of the elements y_{2n} in $\mathrm{gr}^1_{\mathfrak{D}}\mathfrak{dm}_0(\mathbb{Q})$ are zero (which in $\mathfrak{dm}_0(\mathbb{Q})$ follows from [Rac02, Proposition 2.2], but holds in $\mathfrak{ls}$ by Definition 5.3). □

Many thanks to a referee for pointing out at least two places in the literature which have subsequently provided a more detailed proof of this statement: [Maa19] and also [Sch15, Theorem 3.4.3]. It would be interesting to know if a suitable linearized version of the associator relations is equivalent to the linearized double shuffle relations.

5.2 Summary of definitions

We have the following Lie subalgebras of the Lie algebra $\mathfrak{g} \cong (\mathbb{L}(e_0, e_1), \{\,,\})$, equipped with the Ihara bracket:

$$\mathfrak{g}^{\mathfrak{m}} \subseteq \mathfrak{dm}_0(\mathbb{Q}),$$

where $\mathfrak{g}^{\mathfrak{m}}$ is the image of the (weight-graded) Lie algebra of $\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$ and is isomorphic to the free graded Lie algebra on (non-canonical) generators σ_{2i+1} for $i \geq 1$. A standard conjecture states that $\mathfrak{g}^{\mathfrak{m}} \subseteq \mathfrak{dm}_0(\mathbb{Q})$ is an isomorphism. Passing to the depth-graded versions, and writing $\mathfrak{dg}^{\mathfrak{m}} = \mathrm{gr}_{\mathfrak{D}}\mathfrak{g}^{\mathfrak{m}}$, we have inclusions of bigraded Lie algebras

$$\mathfrak{dg}^{\mathfrak{m}} \subseteq \mathrm{gr}_{\mathfrak{D}}\,\mathfrak{dm}_0(\mathbb{Q}) \subseteq \mathfrak{ls}, \tag{5.11}$$

where $\mathfrak{ls}$ stands for the linearized double shuffle algebra. Once again, all Lie algebras in (5.11) are conjectured to be equal. The bigraded dual space $(\mathfrak{dg}^{\mathfrak{m}})^{\vee}$ is isomorphic to the Lie coalgebra of depth-graded motivic multiple zeta values, modulo $\zeta^{\mathfrak{m}}(2)$ and modulo products. The Lie algebras (5.11) are Lie subalgebras of $\mathrm{gr}_{\mathfrak{D}}\mathfrak{g} \cong \mathfrak{g}$, since the Ihara bracket is homogeneous with respect to $\mathfrak{D}$-degree.

All the above Lie algebras can, in particular, be viewed inside the vector space $\mathcal{U}\mathbb{L}(e_0, e_1) = T(\mathbb{Q}e_0 \oplus \mathbb{Q}e_1)$, which is graded for the $\mathfrak{D}$-degree. Next, we show that complicated expressions in the non-commutative algebra $T(\mathbb{Q}e_0 \oplus \mathbb{Q}e_1)$ can be greatly simplified by encoding words of fixed $\mathfrak{D}$-degree in terms of polynomials.

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6. Polynomial representations

6.1 Composition of polynomials

Recall from (2.1) that $\mathcal{U}\,\mathbb{L}(e_0,e_1)$ is isomorphic to the bigraded tensor algebra $T(e_0,e_1)$, and the space $\mathrm{gr}^r_{\mathfrak{D}}\,\mathcal{U}\,\mathbb{L}(e_0,e_1)=\mathrm{gr}^r_{\mathfrak{D}}\,T(e_0,e_1)$ of $\mathfrak{D}$-degree r is the spanned by words in e_0,e_1 with exactly r occurrences of e_1.

Definition 6.1. Consider the isomorphism of vector spaces

$$\begin{aligned}\rho:\mathrm{gr}^r_{\mathfrak{D}}\,T(e_0,e_1)&\longrightarrow\mathbb{Q}[y_0,\ldots,y_r]\\ e_0^{a_0}e_1e_0^{a_1}e_1\ldots e_1e_0^{a_r}&\mapsto y_0^{a_0}y_1^{a_1}\ldots y_r^{a_r}.\end{aligned}\tag{6.1}$$

It maps elements of degree n to elements of degree $n-r$.

The operator $\underline{\circ}:T(e_0,e_1)\otimes_{\mathbb{Q}}T(e_0,e_1)\to T(e_0,e_1)$ respects the $\mathfrak{D}$-grading, so defines a map

$$\begin{aligned}\underline{\circ}:\mathbb{Q}[y_0,\ldots,y_r]\otimes_{\mathbb{Q}}\mathbb{Q}[y_0,\ldots,y_s]&\longrightarrow\mathbb{Q}[y_0,\ldots,y_{r+s}]\\ f(y_0,\ldots,y_r)\otimes g(y_0,\ldots,y_s)&\mapsto f\,\underline{\circ}\,g\,(y_0,\ldots,y_{r+s})\end{aligned}\tag{6.2}$$

which can be read off from (2.7). Explicitly, it is

$$\begin{aligned}f\,\underline{\circ}\,g(y_0,\ldots,y_{r+s})&=\sum_{i=0}^{s}f(y_i,y_{i+1},\ldots,y_{i+r})g(y_0,\ldots,y_i,y_{i+r+1},\ldots,y_{r+s})\\&\quad+(-1)^{\deg f+r}\sum_{i=1}^{s}f(y_{i+r},\ldots,y_{i+1},y_i)g(y_0,\ldots,y_{i-1},y_{i+r},\ldots,y_{r+s}).\end{aligned}\tag{6.3}$$

Antisymmetrizing, and using Proposition 2.2, we obtain a formula for the Ihara bracket

$$\begin{aligned}\mathfrak{g}\wedge\mathfrak{g}&\longrightarrow\mathfrak{g}\\ \{f,g\}&=f\,\underline{\circ}\,g-g\,\underline{\circ}\,f.\end{aligned}\tag{6.4}$$

The linearized double shuffle relations on words translate into functional equations for polynomials after applying the map ρ. We describe some of these below.

6.2 Translation invariance

The additive group $\mathbb{G}_a$ acts on $\mathbb{A}^{r+1}$ by translation, and hence $\mathbb{G}_a(\mathbb{Q})$ acts on its ring of functions via $\lambda:(y_0,\ldots,y_r)\mapsto(y_0+\lambda,\ldots,y_r+\lambda)$.

Lemma 6.2. *The image of $\mathfrak{g}^{\mathfrak{m}}$ under ρ is contained in the subspace of polynomials in $\mathbb{Q}[y_0,\ldots,y_r]$ which are invariant under translation.*

Proof. The subspace $\mathfrak{g}^{\mathfrak{m}}\subset\mathfrak{g}\cong\mathbb{L}(e_0,e_1)\subset T(e_0,e_1)$ is contained in the subspace of elements which are primitive with respect to the shuffle coproduct $\Delta_{ш}$. Let $\pi_0:T(e_0,e_1)\to\mathbb{Q}$ denote the linear map which sends the word e_0 to 1 and all other words to 0, and consider the map $\partial_0=(\pi_0\otimes id)\circ\Delta_{ш}$. It defines a derivation $\partial_0:T(e_0,e_1)\longrightarrow T(e_0,e_1)$ which satisfies

$$\partial_0(e_0^{a_0}e_1\ldots e_1e_0^{a_r})=\sum_{i=0}^{r}a_i\,e_0^{a_0}e_1\ldots e_1e_0^{a_i-1}e_1\ldots e_1e_0^{a_r}$$

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for all non-negative integers $a_0,\dots,a_r$. Let $r\geq 1$, $\xi\in \mathrm{gr}^r_{\mathfrak{D}} T(e_0,e_1)$, and $f=\rho(\xi)$. If ξ is primitive for $\Delta_{\text{ш}}$, it satisfies $\partial_0\xi=0$ and the previous equation is

$$\sum_{i=0}^{r}\frac{\partial f}{\partial y_i}=0. \tag{6.5}$$

This is equivalent to $(\partial/\partial\lambda)g=0$, where $g=f(y_0,\dots,y_r)-f(y_0+\lambda,\dots,y_r+\lambda)$. Therefore g is constant in λ. It vanishes at $\lambda=0$, so $g\equiv 0$ and f is translation invariant. □

Let us denote the map which sends y_0 to zero and y_i to x_i for $i=1,\dots,r$ by

$$\begin{aligned}\mathbb{Q}[y_0,\dots,y_r] &\longrightarrow \mathbb{Q}[x_1,\dots,x_r]\\ f&\mapsto \bar{f},\end{aligned} \tag{6.6}$$

where $\bar{f}$ is the 'reduced' polynomial $\bar{f}(x_1,\dots,x_r)=f(0,x_1,\dots,x_r)$. In the case when f is translation invariant, we can retrieve f from $\bar{f}$ via

$$f(y_0,\dots,y_r)=\bar{f}(y_1-y_0,\dots,y_r-y_0). \tag{6.7}$$

Taking the coefficients of (6.7) gives equation **I2** of [Bro12], which gives a formula for the shuffle-regularization of iterated integrals which begin with any sequence of 0's.

Definition 6.3. For any element $\xi\in\mathfrak{dg}^{\mathfrak{m}}$ of depth r we denote its *reduced* polynomial representation by $\bar{\rho}(\xi)\in\mathbb{Q}[x_1,\dots,x_r]$.

To avoid confusion, we reserve the variables $x_1,\dots,x_r$ for the reduced polynomial $\bar{\rho}(\xi)$ and use the variables $y_0,\dots,y_r$ as above to denote the full polynomial $\rho(\xi)$.

6.3 Antipodal symmetries

The set of primitive elements in a Hopf algebra is stable under the antipode. For the shuffle Hopf algebra this is the map $*: T(e_0,e_1)\to T(e_0,e_1)$ which sends $w\mapsto(-1)^{|w|}\tilde{w}$, where $\tilde{w}$ is the reversed word and $|w|$ the length of w. Restricting to $\mathfrak{D}$-degree r and transporting via ρ, we obtain a map

$$\begin{aligned}\sigma:\mathbb{Q}[y_0,\dots,y_r]&\longrightarrow \mathbb{Q}[y_0,\dots,y_r]\\ \sigma(f)(y_0,\dots,y_r)&=(-1)^{\deg(f)+r}f(y_r,\dots,y_0).\end{aligned} \tag{6.8}$$

Therefore, if $f\in\mathbb{Q}[y_0,\dots,y_r]$ satisfies the shuffle relations (5.3), then

$$f+\sigma(f)=0. \tag{6.9}$$

Since the stuffle algebra, graded for the depth filtration, is isomorphic to the shuffle algebra on Y (5.9), it follows that its antipode is the map $\mathsf{y}_{i_1}\dots\mathsf{y}_{i_r}\mapsto(-1)^r\mathsf{y}_{i_r}\dots\mathsf{y}_{i_1}$. This defines an involution

$$\begin{aligned}\bar{\tau}:\mathbb{Q}[x_1,\dots,x_r]&\longrightarrow\mathbb{Q}[x_1,\dots,x_r]\\ \bar{\tau}(\bar{f})(x_1,\dots,x_r)&=(-1)^r\bar{f}(x_r,\dots,x_1).\end{aligned} \tag{6.10}$$

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Therefore if $\bar{f} \in \mathbb{Q}[x_1, \ldots, x_r]$ satisfies the linearized stuffle relations, then $\bar{f} + \bar{\tau}(\bar{f}) = 0$. Note that the involution $\bar{\tau}$ lifts to an involution

$$\begin{aligned} \tau : \mathbb{Q}[y_0, y_1, \ldots, y_r] &\longrightarrow \mathbb{Q}[y_0, y_1, \ldots, y_r] \\ \tau(f)(y_0, y_1, \ldots, y_r) &= (-1)^r f(y_0, y_r, \ldots, y_1), \end{aligned} \tag{6.11}$$

and therefore if $f \in \mathbb{Q}[y_0, \ldots, y_r]$ satisfies both translational invariance and the linearized stuffle relations, we have

$$f + \tau(f) = 0. \tag{6.12}$$

The composition $\tau\sigma$ is the signed cyclic rotation of order $r+1$,

$$\tau\sigma(f)(y_0, \ldots, y_r) = (-1)^{\deg f} f(y_r, y_0, \ldots, y_{r-1}),$$

and plays an important role in the rest of this paper.

6.4 Parity relations

The following result is well known, and was first proved by Tsumura [Tsu04], and subsequently in ([IKZ06, Theorem 7]). We repeat the proof for convenience.

Proposition 6.4. *The components of $\mathfrak{ls}$ in weight N and depth r vanish unless $N \equiv r$ mod2. Equivalently, $\rho(\mathfrak{ls})$ consists of polynomials of even degree only.*

Proof. Let $f \in \mathbb{Q}[y_0, \ldots, y_r]$ be in the image of $\rho(\mathfrak{dg}_r^{\mathfrak{m}})$. In particular, it satisfies the linearized stuffle relations (6.9) and (6.12). Following [IKZ06], consider the relation

$$\mathsf{y}_1 ш \mathsf{y}_2 \ldots \mathsf{y}_r = \mathsf{y}_1 \ldots \mathsf{y}_r + \sum_{i=2}^{r} \mathsf{y}_2 \ldots \mathsf{y}_i \mathsf{y}_1 \mathsf{y}_{i+1} \ldots \mathsf{y}_r,$$

where $r \geq 2$ (the case $r = 1$ follows from Definition 5.3). Then we have

$$f(y_0, y_1, \ldots, y_r) + \sum_{i=2}^{r} f(y_0, y_2, \ldots, y_i, y_1, y_{i+1}, \ldots, y_r) = 0.$$

Now apply the automorphism of $\mathbb{Q}[y_0, \ldots, y_r]$ defined on generators by $y_i \mapsto y_{i+1}$, where i is taken modulo $r+1$. This leads to the equation

$$f(y_1, y_2, \ldots, y_r, y_0) + \sum_{i=3}^{r+1} f(y_1, y_3, \ldots, y_i, y_2, y_{i+1}, \ldots, y_r, y_0) = 0.$$

By applying a cyclic rotation $\tau\sigma$ to each term, we get

$$f(y_0, y_1, y_2, \ldots, y_r) + \sum_{i=3}^{r} f(y_0, y_1, y_3, \ldots, y_i, y_2, y_{i+1}, \ldots, y_r) + f(y_2, y_1, y_3, \ldots, y_r, y_0) = 0.$$

The first two terms can be interpreted as the terms occurring in the linearized stuffle product $(\mathsf{y}_2 ш \mathsf{y}_1 \mathsf{y}_3 \ldots \mathsf{y}_r)$ minus the first term. As a result, one obtains the equation

$$-f(y_0, y_2, y_1, y_3, \ldots, y_r) + f(y_2, y_1, y_3, \ldots, y_r, y_0) = 0,$$

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which, by a final application of $\tau\sigma$ to the right-hand term, yields

$$((-1)^{\deg f} - 1) f(y_0, y_2, y_1, y_3, \ldots, y_r) = 0.$$

Therefore, in the case when $\deg f$ is odd, the polynomial f must vanish. □

6.5 Dihedral symmetry and the Ihara bracket

For all $r \geq 1$, consider the graded vector space $\mathfrak{p}_r$ of polynomials $f \in \mathbb{Q}[y_0, \ldots, y_r]$ which satisfy

$$\begin{gathered} f(y_0, \ldots, y_r) = f(-y_0, \ldots, -y_r), \\ f + \sigma(f) = f + \tau(f) = 0. \end{gathered} \tag{6.13}$$

The maps σ, τ generate a dihedral group $D_{r+1} = \langle \sigma, \tau \rangle$ of symmetries acting on $\mathfrak{p}_r$ of order $2r+2$, and any element f satisfying (6.13) is invariant under cyclic rotation:

$$f = \sigma\tau(f), \quad \text{where } (\sigma\tau)^{r+1} = id,$$

and anti-invariant under the reflections σ and τ. Thus $\mathbb{Q}f \subset \mathfrak{p}_r$ is isomorphic to the one-dimensional sign (orientation) representation ε of the dihedral group D_{r+1}.

Proposition 6.5. *Suppose that $f \in \mathfrak{p}_r$ and $g \in \mathfrak{p}_s$ are polynomials satisfying (6.13). Then the Ihara bracket is the signed average over the dihedral symmetry group:*

$$\{f, g\} = \sum_{\mu \in D_{r+s+1}} \varepsilon(\mu) \mu\big(f(y_0, y_1, \ldots, y_r) g(y_r, y_{r+1} \ldots, y_{r+s})\big). \tag{6.14}$$

In particular, $\{.,.\} : \mathfrak{p}_r \times \mathfrak{p}_s \to \mathfrak{p}_{r+s}$, and $\mathfrak{p} = \bigoplus_{r \geq 1} \mathfrak{p}_r$ is a bigraded Lie algebra.

Proof. A straightforward calculation from (6.3) and definition (6.4) gives

$$\{f, g\} = \sum_i f(y_i, y_{i+1}, \ldots, y_{i+r}) \big(g(y_{i+r}, y_{i+r+1}, \ldots, y_{i-1}) - g(y_{i+r+1}, y_{i+r+2}, \ldots, y_i)\big),$$

where the summation indices are taken modulo $r+s+1$. Invoking dihedral symmetry of f, g leads to formula (6.14). The Jacobi identity for $\{.,.\}$ is automatic since the Ihara action is an action, but can also be proved very easily by identifying its terms with the set of double cuts in a polygon (see [Bro17b]). The fact that parity (first equation of (6.13)) is preserved by $\{\,,\}$ is clear. The anti-invariance under σ, τ is also clear from the dihedral symmetry of (6.14). □

A similar dihedral symmetry was also found by Goncharov [Gon01b]; the interpretation of the dihedral reflections as antipodes may or may not be new. Since the Ihara action is, by definition, compatible with the shuffle product, it follows from Lemma 6.2 that translation invariance is preserved by the Ihara bracket. One can also easily verify this by direct computation:

$$\sum_{i=0}^{r} \frac{\partial f}{\partial y_i} = \sum_{i=0}^{s} \frac{\partial g}{\partial y_i} = 0 \quad \Longrightarrow \quad \sum_{i=0}^{r+s} \frac{\partial \{f, g\}}{\partial y_i} = 0.$$

Definition 6.6. Let $\bar{\mathfrak{p}}_r \subset \mathfrak{p}_r$ denote the subspace of polynomials which satisfy (6.13) and are invariant under translation, and write $\bar{\mathfrak{p}} = \bigoplus_{r \geq 1} \bar{\mathfrak{p}}_r$.

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By abuse of notation, we can equivalently view $\bar{\mathfrak{p}}_r$ as the subspace of polynomials $\bar{f} \in \mathbb{Q}[x_1, \dots, x_r]$ whose lift $\bar{f}(y_1 - y_0, \dots, y_r - y_0)$ lies in $\mathfrak{p}_r$. Explicitly, $\bar{\mathfrak{p}}_r$ is the vector space of polynomials satisfying

(1) $\bar{f}(x_1, \dots, x_r) = \bar{f}(-x_1, \dots, -x_r)$,
(2) $\bar{f}(x_1, \dots, x_r) + (-1)^r \bar{f}(x_r, \dots, x_1) = 0$,
(3) $\bar{f}(x_1, \dots, x_r) + (-1)^r \bar{f}(x_{r-1} - x_r, \dots, x_1 - x_r, -x_r) = 0$,

with Lie bracket induced by (6.14). To conclude the previous discussion, the map

$$\bar{\rho} : \mathfrak{dg}^{\mathfrak{m}} \longrightarrow \bar{\mathfrak{p}}$$

is an injective map of bigraded Lie algebras.

Definition 6.7. We use the notation $\mathbb{D}_r \subset \mathbb{Q}[x_1, \dots, x_r]$ to denote the space $\bar{\rho}(\mathfrak{ls}_r)$ in depth r. It is the space of polynomial solutions to the linearized double shuffle equations in depth r and is the direct sum for all n, of spaces denoted $D_{n,r}$ in [IKZ06].

6.6 Generators in depth 1 and examples

It follows from Theorem 1.1 that in depth 1, the Lie algebra $\mathfrak{dg}^{\mathfrak{m}}$ has exactly one generator in every odd weight ≥ 3:

$$\bar{\rho}(\mathfrak{dg}_1^{\mathfrak{m}}) = \bigoplus_{n \geq 1} \mathbb{Q}\, x_1^{2n}.$$

In particular, the algebras $\mathfrak{dg}^{\mathfrak{m}} \subset \mathrm{gr}_{\mathfrak{D}} \mathfrak{dm}_0(\mathbb{Q}) \subset \mathfrak{ls}$ are all isomorphic in depth 1.

Definition 6.8. Denote the Lie subalgebra generated by x_1^{2n}, for $n \geq 1$, by

$$\mathfrak{dg}^{\mathrm{odd}} \subset \mathfrak{dg}^{\mathfrak{m}}. \tag{6.15}$$

Example 6.9. The formula for the Ihara bracket in depth 2 can be written

$$\{x_1^{2m}, x_1^{2n}\} = x_1^{2m}\big(x_2^{2n} - (x_2 - x_1)^{2n}\big) + (x_2 - x_1)^{2m}\big(x_1^{2n} - x_2^{2n}\big) + x_2^{2m}\big((x_2 - x_1)^{2n} - x_1^{2n}\big).$$

6.7 Relations between depth-graded motivic multiple zeta values

We briefly explain how we may describe all relations between $\zeta_{\mathfrak{D}}^{\mathfrak{m}}$ using this formalism.

Proposition 4.2 states that $\mathrm{gr}^{\mathfrak{D}} \mathcal{H}$ is the free bigraded right $\mathcal{U}\mathfrak{dg}^{\mathfrak{m}}$-module generated by the $\zeta_{\mathfrak{D}}^{\mathfrak{m}}(2n)$, and can be represented by polynomials as follows. The role of the even zeta value $\zeta^{\mathfrak{m}}(2n)$, for $n \geq 1$, is played by the depth-graded associator element $\tau^{(1)}$ in weight $2n$ constructed in [Bro17a, §§ 7.3 and 7.4], and is encoded by the monomial in one variable:

$$\bar{\tau}_{2n} = x_1^{2n-1}.$$

Therefore, a relation

$$\sum_{n_1 + \dots + n_d = N} \lambda_{n_1, \dots, n_d}\, \zeta_{\mathfrak{D}}^{\mathfrak{m}}(n_1, \dots, n_d) = 0$$

holds between (shuffle-regularized) depth-graded motivic multiple zeta values in depth d and weight N if and only if $\sum_{\underline{n} = (n_1, \dots, n_d)} \lambda_{\underline{n}} c_{\underline{n}} = 0$ for all

$$\xi = \sum_{n_1 + \dots + n_d = N} c_{n_1, \dots, n_d}\, x_1^{n_1 - 1} \dots x_d^{n_d - 1},$$

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where ξ is of depth d and weight N of the form

$$x = g_1 \,\underline{\circ}\, \big(g_2 \,\underline{\circ}\, \big(\ldots\ldots \big(g_{d-1} \,\underline{\circ}\, g_d\big)\cdots\big)\big) \quad \text{if } N \equiv d \pmod 2,$$
$$x = g_1 \,\underline{\circ}\, \big(g_2 \,\underline{\circ}\, \big(\ldots\ldots \big(g_{d-1} \,\underline{\circ}\, \bar{\tau}_{2k}\big)\cdots\big)\big) \quad \text{if } N \not\equiv d \pmod 2,$$

in which the g_i are the polynomial representatives of generators of $\mathfrak{dg}^{\mathfrak{m}}$ and $k \geq 1$.

Example 6.10. We give some simple examples in depth 2. For this, our formula for $\underline{\circ}$ gives, for any $m, n \geq 1$,

$$x_1^{2m} \,\underline{\circ}\, x_1^n = x_1^{2m} x_2^n + (x_2 - x_1)^{2m}\big(x_1^n - x_2^n\big). \tag{6.16}$$

(1) In weight 5, depth 2, $\mathrm{gr}_2^{\mathfrak{D}}\mathcal{H}_5$ is one-dimensional generated by the element $\bar{\sigma}_3 \circ \bar{\tau}_2$, which we can compute using (6.16) to be

$$x_1^2 \,\underline{\circ}\, x_1 = x_1^3 - 2x_1^2 x_2 + 3x_1 x_2^2 - x_2^3.$$

It encodes the coefficients of $\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(2)$ in the following (shuffle-regularized) depth-graded multiple zeta values in depth 2 and weight 4, as one can see from the relations

$$\begin{aligned}
\zeta^{\mathfrak{m}}(3,2) &= \tfrac{9}{2}\,\zeta^{\mathfrak{m}}(5) - 2\,\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(2),\\
\zeta^{\mathfrak{m}}(2,3) &= -\tfrac{11}{2}\,\zeta^{\mathfrak{m}}(5) + 3\,\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(2),\\
\zeta^{\mathfrak{m}}(1,4) &= 2\,\zeta(5) - \zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}2).
\end{aligned}$$

For instance, we may read off the relation $3\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,2) + 2\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2,3) = 0$ from $x_1^2 \,\underline{\circ}\, x_1$.

(2) In weight 7, depth 2, $\mathrm{gr}_2^{\mathfrak{D}}\mathcal{H}_7$ is two-dimensional generated by the two elements $\bar{\sigma}_5 \circ \bar{\tau}_2$ and $\bar{\sigma}_3 \circ \bar{\tau}_4$, which we compute via

$$\begin{aligned}
x_1^4 \,\underline{\circ}\, x_1 &= x_1^5 - 4\,x_1^4 x_2 + 10\,x_1^3 x_2^2 - 10\,x_1^2 x_2^3 + 5\,x_1 x_2^4 - x_2^5\\
x_1^2 \,\underline{\circ}\, x_1^3 &= x_1^5 - 2\,x_1^4 x_2 + x_1^3 x_2^2 + 2\,x_1 x_2^4 - x_2^5.
\end{aligned}$$

The coefficients in these expressions encode the coefficients of $\zeta^{\mathfrak{m}}(5)\zeta^{\mathfrak{m}}(2)$ and $\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(4)$ in depth 2 multiple zeta values of weight 7. For example,

$$\begin{aligned}
\zeta^{\mathfrak{m}}(5,2) &= 10\,\zeta^{\mathfrak{m}}(7) - 4\,\zeta^{\mathfrak{m}}(5)\zeta^{\mathfrak{m}}(2) - 2\,\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(4),\\
\zeta^{\mathfrak{m}}(4,3) &= -18\,\zeta^{\mathfrak{m}}(7) + 10\,\zeta^{\mathfrak{m}}(5)\zeta^{\mathfrak{m}}(2) + \zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(4),\\
\zeta^{\mathfrak{m}}(3,4) &= 17\,\zeta^{\mathfrak{m}}(7) - 10\,\zeta^{\mathfrak{m}}(5)\zeta^{\mathfrak{m}}(2),\\
\zeta^{\mathfrak{m}}(2,5) &= -11\,\zeta^{\mathfrak{m}}(7) + 5\,\zeta^{\mathfrak{m}}(5)\zeta^{\mathfrak{m}}(2) + 2\,\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(4).
\end{aligned}$$

Choosing any linear functional on the coefficients of $x_1^4 x_2$, $x_1^3 x_2^2$ and $x_1^2 x_2^3$ which vanishes on $x_1^4 \,\underline{\circ}\, x_1$ and $x_1^2 \,\underline{\circ}\, x_1^3$ leads to a relation between depth-graded motivic multiple zeta values, for instance:

$$\zeta^{\mathfrak{m}}_{\mathfrak{D}}(5,2) + 2\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(4,3) + \tfrac{8}{5}\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,4) = 0.$$

(3) In weight 8, depth 2, $\mathrm{gr}_2^{\mathfrak{D}}\mathcal{H}_8$ is two-dimensional generated by the pair of elements $\bar{\sigma}_3 \circ \bar{\sigma}_5$ and $\bar{\sigma}_5 \circ \bar{\sigma}_3$, which we compute using (6.16) by

$$\begin{aligned}
x_1^4 \,\underline{\circ}\, x_1^2 &= x_1^6 - 2\,x_1^5 x_2 + x_1^4 x_2^2 + 2\,x_1 x_2^5 - x_2^6\\
x_1^2 \,\underline{\circ}\, x_1^4 &= x_1^6 - 4\,x_1^5 x_2 + 6\,x_1^4 x_2^2 - 5\,x_1^2 x_2^4 + 4\,x_1 x_2^5 - x_2^6.
\end{aligned}$$

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From these, we deduce all relations between depth-graded motivic multiple zeta values of weight 8 and depth 2, such as

$$2\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,5)+5\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2,6)+10\,\zeta^{\mathfrak{m}}_{\mathfrak{D}}(1,7)=0$$

since $2.(0)+5.(2)+10.(-1)=0$ and $2.(-5)+5.(4)+10.(-1)=0$ where the numbers in brackets are the coefficients of $x_1^2x_2^4$, $x_1x_2^5$, x_2^6 in $x_1^4\,\underline{\circ}\,x_1^2$ and $x_1^2\,\underline{\circ}\,x_3^2$. Indeed, one may check that $5\,\zeta^{\mathfrak{m}}(2,6)+2\,\zeta^{\mathfrak{m}}(3,5)+10\,\zeta^{\mathfrak{m}}(1,7)=\frac{6}{175}\zeta^{\mathfrak{m}}(2)^4$.

7. Modular relations in depth 2

7.1 Reminders on period polynomials

We recall some definitions from [KZ84, § 1.1]. Let $S_{2k}(\mathrm{SL}_2(\mathbb{Z}))$ denote the space of cusp forms of weight $2k$ for the full modular group $\mathrm{SL}_2(\mathbb{Z})$.

Definition 7.1. Let $n\geq 1$ and let $W^e_{2n}\subset\mathbb{Q}[X,Y]$ denote the vector space of homogeneous polynomials $P(X,Y)$ of degree $2n-2$ satisfying

$$P(X,Y)+P(Y,X)=0,\quad P(\pm X,\pm Y)=P(X,Y), \tag{7.1}$$

$$P(X,Y)+P(X-Y,X)+P(-Y,X-Y)=0. \tag{7.2}$$

The space W^e_{2n} contains the polynomial $p_{2n}=X^{2n-2}-Y^{2n-2}$, and is a direct sum

$$W^e_{2n}\cong\mathsf{S}_{2n}\oplus\mathbb{Q}\,p_{2n},$$

where S_{2n} is the subspace of polynomials which vanish at $(X,Y)=(1,0)$. We write $\mathsf{S}=\bigoplus_n\mathsf{S}_{2n}$. The Eichler–Shimura–Manin theorem gives a map which associates, in particular, an even-period polynomial to every cusp form:

$$S_{2k}(\mathrm{SL}_2(\mathbb{Z}))\longrightarrow W^e_{2k}\otimes_{\mathbb{Q}}\mathbb{C}.$$

Explicitly, if f is a cusp form of weight $2k$, the map is given by

$$f\quad\mapsto\quad\left(\int_0^{i\infty}f(z)(X-zY)^{2k-2}\,dz\right)^+, \tag{7.3}$$

where $+$ denotes the projection onto invariants under the involution $(X,Y)\mapsto(X,-Y)$, that is, $a^+(X,Y)=\frac{1}{2}(a(X,Y)+a(X,-Y))$. The three-term equation (7.2) follows from integrating around the geodesic triangle with vertices $0,1,i\infty$ and is reminiscent of the hexagon equation for associators. The map (7.3) is an isomorphism onto a subspace of $W^e_{2k}\otimes\mathbb{C}$ of codimension 1. Thus $\dim S_{2k}(\mathrm{SL}_2(\mathbb{Z}))=\dim\mathsf{S}_{2k}$ and it follows from classical results on the space of modular forms of level 1 that

$$\sum_{n\geq 0}\dim\mathsf{S}_{2n}s^{2n}=\frac{s^{12}}{(1-s^4)(1-s^6)}=\mathbb{S}(s). \tag{7.4}$$

7.2 Linearized double shuffle in depths 2 and 3

We first recall from [IKZ06] that $\mathbb{D}_2$ is the graded space of homogeneous polynomials $f\in\mathbb{Q}[x_1,x_2]$ in two variables satisfying the linearized double shuffle equations in depth 2:

$$f(x_1,x_2)+f(x_2,x_1)=0\quad\text{and}\quad f(x_1,x_1+x_2)+f(x_2,x_1+x_2)=0.$$

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The space $\mathbb{D}_3$ consists of homogeneous polynomials $f \in \mathbb{Q}[x_1, x_2, x_3]$ such that

$$f(x_1, x_2, x_3) + f(x_2, x_1, x_3) + f(x_2, x_3, x_1) = 0,$$
$$f^\sharp(x_1, x_2, x_3) + f^\sharp(x_2, x_1, x_3) + f^\sharp(x_2, x_3, x_1) = 0,$$

where $f^\sharp(x, y, z) = f(x, x + y, x + y + z)$. The general double shuffle equations and their linearized versions are derived in [Bro17b, §§ 4–7] using Hopf-algebra-theoretic techniques.

7.3 A short exact sequence in depth 2

The Ihara bracket gives a map

$$\{\,,\} : \mathfrak{ls}_1 \wedge \mathfrak{ls}_1 \longrightarrow \mathfrak{ls}_2. \tag{7.5}$$

Applying the isomorphism $\bar{\rho}$ leads to a map

$$\mathbb{D}_1 \wedge \mathbb{D}_1 \longrightarrow \mathbb{D}_2, \tag{7.6}$$

given by the formula in Example 6.9. Since $\mathbb{D}_1$ is isomorphic to the graded vector space $\mathbb{Q}[x_1^{2n}, n \geq 1]$, it follows that $\mathbb{D}_1 \wedge \mathbb{D}_1$ is isomorphic to the space of antisymmetric even polynomials $p(x_1, x_2)$ with positive bidegrees, with basis $x_1^{2m} x_2^{2n} - x_1^{2n} x_2^{2m}$ for $m > n > 0$. It follows from Example 6.9 that the image of $p(x_1, x_2)$ under (7.6) is

$$p(x_1, x_2) + p(x_2 - x_1, x_1) + p(-x_2, x_1 - x_2).$$

Comparing with (7.2) and (7.1), we immediately deduce (cf. [IT93, Gon05, GKZ06, Sch06]) that

$$\ker(\{\,,\} : \mathbb{D}_1 \wedge \mathbb{D}_1 \longrightarrow \mathbb{D}_2) \xrightarrow{\sim} \mathsf{S}. \tag{7.7}$$

In fact, the dimensions of the space $\mathbb{D}_2$ have been computed several times in the literature (e.g. by some simple representation-theoretic arguments), and it is relatively easy to show [GKZ06] that the following sequence is exact:

$$0 \longrightarrow \mathsf{S} \longrightarrow \mathbb{D}_1 \wedge \mathbb{D}_1 \longrightarrow \mathbb{D}_2 \longrightarrow 0. \tag{7.8}$$

Example 7.2. The smallest non-trivial period polynomial occurs in degree 10 and is given by $s_{12} = X^2Y^2(X - Y)^3(X + Y)^3 = X^8Y^2 - 3X^6Y^4 + 3X^4Y^6 - X^2Y^8$. By the exact sequence (7.8) it immediately gives rise to the equation

$$3\{x_1^4, x_1^6\} = \{x_1^2, x_1^8\}, \tag{7.9}$$

which, by the faithfulness of the map $\bar{\rho}$, is equivalent to Ihara's formula (1.7).

7.4 A short exact sequence in depth 3

If V is a vector space let $\mathrm{Lie}_n(V) \subset V^{\otimes n}$ denote the component of degree n in the free graded Lie algebra $\mathrm{Lie}(V)$ generated by V, viewed inside the tensor algebra $T(V) = \bigoplus_{n\geq 0} V^{\otimes n}$. It is the subspace spanned by Lie brackets of the form $[v_1, [v_2, \ldots, [v_{n-1}, v_n] \ldots]$ where the Lie bracket on $T(V)$ is the antisymmetrization of the tensor multiplication (i.e.$[v_1, v_2] = v_1v_2 - v_2v_1$). Thus, as a graded vector space, $\mathrm{Lie}(V) \cong \bigoplus_{n\geq 1} \mathrm{Lie}_n(V)$, and each Lie_n is a direct sum of Schur functors (e.g. $\mathrm{Lie}_1(V) = V$ and $\mathrm{Lie}_2(V) = \bigwedge^2 V$).

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The triple Ihara bracket gives a trilinear map

$$\mathrm{Lie}_3(\mathfrak{ls}_1) \longrightarrow \mathfrak{ls}_3,$$

and hence a map $\mathrm{Lie}_3(\mathbb{D}_1) \to \mathbb{D}_3$ whose image is spanned by $\{x_1^{2a}, \{x_1^{2b}, x_1^{2c}\}\}$, for $a, b, c \geq 1$. Goncharov has studied the space $\mathbb{D}_3$, and computed its dimensions in each weight [Gon05]. It follows from his work that the sequence

$$0 \longrightarrow \mathsf{S} \otimes_{\mathbb{Q}} \mathbb{D}_1 \longrightarrow \mathrm{Lie}_3(\mathbb{D}_1) \longrightarrow \mathbb{D}_3 \longrightarrow 0 \tag{7.10}$$

is exact, where the first map (identifying S with $\ker(\Lambda^2\mathbb{D}_1 \to \mathbb{D}_2)$) is given by

$$\mathsf{S} \otimes_{\mathbb{Q}} \mathbb{D}_1 \hookrightarrow \Lambda^2\mathbb{D}_1 \otimes_{\mathbb{Q}} \mathbb{D}_1 \to \mathrm{Lie}_3(\mathbb{D}_1),$$

and the second map in the sequence immediately above is $[a, b] \otimes c \mapsto [c, [a, b]]$. Starting from depth 4, the structure of $\mathfrak{ls}_d \cong \mathbb{D}_d$ is not known.[6] In particular, it is easy to show that the map given by the quadruple Ihara bracket

$$\mathrm{Lie}_4(\mathbb{D}_1) \longrightarrow \mathbb{D}_4$$

is not surjective, since in weight 12, $\dim \mathbb{D}_4 = 1$, but $\mathrm{Lie}_4(\mathbb{D}_1) = 0$. Our next purpose is to construct the missing elements in depth 4.

Remark 7.3. A different way to think about the sequence (7.10) is via the curious equality $\dim \mathsf{S} \otimes_{\mathbb{Q}} \mathbb{D}_1 = \dim \Lambda^3(\mathbb{D}_1)$ which follows from (7.4). I do not know if there is an appropriate combinatorial or modular interpretation of this identity which could be relevant to the previous exact sequence.

8. Exceptional modular elements in depth 4

8.1 Linearized equations in depth 4

For the convenience of the reader, we write out the linearized double shuffle relations in full in depth 4. There are four equations. In order to write them down we shall use the following notation, where $f \in \mathbb{Q}[x_1, \dots, x_4]$, and we are given any set of indices $\{i, j, k, l\} = \{1, 2, 3, 4\}$:

$$\begin{aligned} f(ijkl) &= f(x_i, x_j, x_k, x_l), \\ f^\sharp(ijkl) &= f(x_i, x_i + x_j, x_i + x_j + x_k, x_i + x_j + x_k + x_l). \end{aligned} \tag{8.1}$$

Then $\mathbb{D}_4$ (see [IKZ06, § 8]) is the subspace of polynomials $f \in \mathbb{Q}[x_1, \dots, x_4]$ satisfying

$$f(1 ш 234) = 0, \quad f(12 ш 34) = 0, \tag{8.2}$$

$$f^\sharp(1 ш 234) = 0, \quad f^\sharp(12 ш 34) = 0, \tag{8.3}$$

where f and $f^\sharp$ are extended by linearity in the obvious way, and

$$1 ш 234 = 1234 + 2134 + 2314 + 2341,$$

$$12 ш 34 = 1234 + 1324 + 1342 + 3124 + 3142 + 3412.$$

[6] After I wrote the first version of this paper, S. Yasuda kindly sent me his private notes [Yas06] in which he gives a conjectural group-theoretic interpretation for the dimensions of $\mathbb{D}_4$, in accordance with the Broadhurst–Kreimer conjecture.

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For example, the first equation of (8.2) is simply

$$f(x_1,x_2,x_3,x_4)+f(x_2,x_1,x_3,x_4)+f(x_2,x_3,x_1,x_4)+f(x_2,x_3,x_4,x_1)=0.$$

We construct some exceptional solutions to these equations from period polynomials.

8.2 Definition of the exceptional elements

Let $f(x,y)\in \mathsf{S}_{2n+2}$ be an even-period polynomial of degree $2n$ which vanishes at $y=0$. It follows from (7.1) and (7.2) that it vanishes along $x=0$ and $x-y=0$. Therefore we can write

$$f(x,y)=xy(x-y)f_0(x,y),$$

where $f_0(x,y)\in\mathbb{Q}[x,y]$ is symmetric and homogeneous of degree $2n-3$, and satisfies

$$f_0(x,y)+f_0(y-x,-x)+f_0(-y,x-y)=0. \tag{8.4}$$

Let us also write $f_1(x,y)=(x-y)f_0(x,y)$. We have $f_1(-x,y)=f_1(x,-y)=-f_1(x,y)$.

Definition 8.1. Let $f\in\mathbb{Q}[x,y]$ be an even-period polynomial as above. Define

$$\begin{aligned}&\mathsf{e}_f\in\mathbb{Q}[y_0,y_1,y_2,y_3,y_4],\\ &\mathsf{e}_f=\sum_{\mathbb{Z}/5\mathbb{Z}}\big(f_1(y_4-y_3,y_2-y_1)+(y_0-y_1)f_0(y_2-y_3,y_4-y_3)\big),\end{aligned} \tag{8.5}$$

where the sum is over cyclic permutations $(y_0,y_1,y_2,y_3,y_4)\mapsto(y_1,y_2,y_3,y_4,y_0)$. Its reduction $\bar{\mathsf{e}}_f\in\mathbb{Q}[x_1,\dots,x_4]$ is obtained by setting $y_0=0, y_i=x_i$, for $i=1,\dots,4$.

Remark 8.2. The full expression for $\bar{e}_f$ is explicitly

$$\begin{aligned}\bar{e}_f(x_1,x_2,x_3,x_4)=\;&f_1(x_4-x_3,x_2-x_1)+f_1(-x_4,x_3-x_2)+f_1(x_1,x_4-x_3)\\ &+f_1(x_2-x_1,-x_4)+f_1(x_3-x_2,x_1)-x_1f_0(x_2-x_3,x_4-x_3)\\ &+(x_1-x_2)f_0(x_3-x_4,-x_4)+(x_2-x_3)f_0(x_4,x_1)\\ &+(x_3-x_4)f_0(-x_1,x_2-x_1)+x_4f_0(x_1-x_2,x_3-x_2).\end{aligned} \tag{8.6}$$

Since f is even it vanishes to order 2 along $x=0,y=0,x=y$. Therefore

$$f_0(0,y)=f_0(x,0)=f_0(x,x)=0,$$

and the same holds *a fortiori* for f_1. If we set $x_3=x_4=0$ in equation (8.6) then all terms except for the fifth vanish and we are left with

$$\bar{\mathsf{e}}_f(x,y,0,0)=f_1(-y,x)=f_1(x,y). \tag{8.7}$$

In this way, the period polynomial f can be retrieved from $\bar{\mathsf{e}}_f$: it is $xy\bar{\mathsf{e}}_f(x,y,0,0)$. This computation is related to the discussion in [BBV10, § 9.2], regarding multiple zeta values of depth 4 of the form $\zeta(1,1,m,n)$.

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8.3 Exceptional elements and linearized double shuffle equations

THEOREM 8.3. *The reduced polynomial* $\bar{\mathsf{e}}_f$ *obtained from* (8.5) *satisfies the linearized double shuffle relations. In particular, we have an injective linear map*

$$\bar{\mathsf{e}} : \mathsf{S} \longrightarrow \mathbb{D}_4.$$

Proof. The injectivity follows immediately from (8.7). The proof that the linearized double shuffle relations hold is a finite computation. In the absence of a purely conceptual proof, we shall break the calculation into more easily verifiable pieces.

We first consider the stuffle equations. It follows from general properties of the Dynkin operator on shuffle algebras that a homogeneous polynomial in four variables satisfies the two linearized stuffle equations (8.2) if and only if it is in the image of the map $\lambda : \mathbb{Q}[x_1, \dots, x_4] \rightarrow \mathbb{Q}[x_1, \dots, x_4]$, with eight terms defined by

$$\lambda(f)(x_1, \dots, x_4) = \alpha(f)(x_1, x_2, x_3, x_4) - \alpha(f)(x_4, x_3, x_2, x_1),$$

where $\alpha(f)(x_1, \dots, x_4)$ is the linear combination

$$f(x_1, x_2, x_3, x_4) - f(x_1, x_2, x_4, x_3) - f(x_1, x_4, x_2, x_3) + f(x_1, x_4, x_3, x_2).$$

For a detailed discussion and proofs, we refer to [Bro17b, § 16.4 and Corollary 16.6]. The linearized stuffle relations (8.2) hold for the sum of the first five terms in f_1, and for the sum of the second five terms in f_0 in (8.6) separately. Consider first the terms in f_1. They consist of two parts:

$$T_1 = f_1(x_4 - x_3, x_2 - x_1)$$

and

$$T_2 = f_1(-x_4, x_3 - x_2) + f_1(x_1, x_4 - x_3) + f_1(x_2 - x_1, -x_4) + f_1(x_3 - x_2, x_1).$$

One easily checks that $\lambda(T_1) = 4\,T_1$, and that $\lambda(f_1(x_1, x_2 - x_3))$ equals

$$\begin{aligned} &f_1(x_1, x_2 - x_3) - f_1(x_1, x_2 - x_4) - f_1(x_1, x_4 - x_2) + f_1(x_1, x_4 - x_3) \\ &\quad - f_1(x_4, x_3 - x_2) + f_1(x_4, x_3 - x_1) + f_1(x_4, x_1 - x_3) - f_1(x_4, x_1 - x_2) = 4\,T_2, \end{aligned}$$

using only the fact that f_1 is antisymmetric and odd in x and y. Thus T_1, T_2 lie in the image of λ and are solutions to the linearized stuffle equations.

Now consider the terms in f_0 in (8.6). Once again, they break into two parts:

$$T_3 = x_4 f_0(x_1 - x_2, x_3 - x_2) - x_1 f_0(x_2 - x_3, x_4 - x_3)$$

and

$$T_4 = (x_1 - x_2) f_0(x_3 - x_4, -x_4) + (x_2 - x_3) f_0(x_4, x_1) + (x_3 - x_4) f_0(-x_1, x_2 - x_1).$$

One checks that $\lambda(T_k) = 4\,T_k$ for $k = 3, 4$ using the three-term relation (8.4), and hence T_3, T_4 are solutions to the linearized stuffle equations. This is the only point in the proof where the three-term relation is needed.

For the linearized shuffle relations, note that there exists $g \in \mathbb{Q}[x, y]$ such that $f_0(x, y) = (x + y) g(x, y)$ and $f_1 = (x^2 - y^2) g(x, y)$ since an even-period polynomial $f(x, y)$ vanishes along $x = y$ and is even in both x and y. The polynomial $g(x, y)$ is symmetric and odd in x and in y (i.e. $g(x, y) = g(y, x)$ and $g(-x, y) = g(x, -y) = -g(x, y)$). These properties suffice to prove that

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(8.6) satisfies the shuffle equations. The full expression again splits into two pieces with four and six terms, respectively:

$$T_5 = (x_4^2 - x_{23}^2)g(x_4, x_{23}) + x_{23}(x_1 + x_4)g(x_1, x_4) + x_{12}(x_{34} - x_4)g(x_{34}, -x_4) \\ + (x_{12}^2 - x_4^2)g(x_{12}, x_4),$$

where we use the notation $x_{ij} = x_i - x_j$, and

$$T_6 = x_{34}(x_{21} - x_1)g(x_1, x_{12}) + x_4(x_{32} + x_{12})g(x_{12}, x_{32}) + (x_{32}^2 - x_1^2)g(x_{32}, x_1) \\ + (x_1^2 - x_{43}^2)g(x_1, x_{43}) + x_1(x_{34} + x_{32})g(x_{32}, x_{34}) + (x_{43}^2 - x_{21}^2)g(x_{43}, x_{21}).$$

Both T_5 and T_6 can laboriously be verified to satisfy the two shuffle equations in depth 4. The statement follows since e_f equals $T_1 + T_2 + T_3 + T_4 = T_5 + T_6$. □

Identifying $\mathfrak{ls}_4$ with $\mathbb{D}_4$ via the map $\bar{\rho}$, we can view e as a map from S to $\mathfrak{ls}_4$. Note that relation (7.2) is proved for the periods of modular forms by integrating round contours very similar to those which prove the symmetry and hexagonal relations for associators. It would be very interesting to see if there is any connection between the five-fold symmetry of the element e_f and the pentagon equation.

Example 8.4. It follows from (7.4) that the space of period polynomials in degrees 12, 16, 18 and 20 is of dimension 1. Choose integral generators:

$$\begin{aligned} f_{12} &= [x_1^8, x_2^2] - 3\,[x_1^6, x_2^4], \\ f_{16} &= 2\,[x_1^{12}, x_2^2] - 7\,[x_1^{10}, x_2^4] + 11\,[x_1^8, x_2^6], \\ f_{18} &= 8\,[x_1^{14}, x_2^2] - 25\,[x_1^{12}, x_2^4] + 26\,[x_1^{10}, x_2^6], \\ f_{20} &= 3\,[x_1^{16}, x_2^2] - 10\,[x_1^{14}, x_2^4] + 14\,[x_1^{12}, x_2^6] - 13\,[x_1^{10}, x_2^8], \end{aligned}$$

where $[x_1^a, x_2^b]$ denotes $x_1^a x_2^b - x_1^b x_2^a$. Let $\mathsf{e}_{12}, \ldots, \mathsf{e}_{20}$ denote the corresponding exceptional elements. We know by Theorem 1.1 that $\mathfrak{g}^{\mathfrak{m}}$ is of dimension 2 in weight 12, spanned by $\{\sigma_3, \sigma_9\}$ and $\{\sigma_5, \sigma_7\}$. We know by (7.9) that in weight 12, $\mathfrak{dg}_2^{\mathfrak{m}}$ is of dimension 1, $\mathfrak{dg}_3^{\mathfrak{m}}$ vanishes by parity, so it follows that $\mathfrak{dg}_4^{\mathfrak{m}}$ is of dimension 1 and hence spanned by $\bar{\mathsf{e}}_{12}$ (since we know that $\mathfrak{ls}_4$ in weight 12 is one-dimensional). Writing out just a few of its coefficients as an example, we have:

$$\bar{\mathsf{e}}_{12} = x_3^7 x_4 - 116\, x_1^3 x_2^2 x_3^2 x_4 - 57\, x_1^2 x_2^5 x_4 + \cdots \quad \text{(118 terms in total)}.$$

Using $\bar{\mathsf{e}}_{12}$, one can write all depth-graded motivic multiple zeta values of depth 4 and weight 12 as multiples of $\zeta_{\mathfrak{D}}(1,1,8,2)$. For example, one has

$$\zeta_{\mathfrak{D}}(4,3,3,2) \equiv -116\,\zeta_{\mathfrak{D}}(1,1,8,2), \quad \zeta_{\mathfrak{D}}(3,6,1,2) \equiv -57\,\zeta_{\mathfrak{D}}(1,1,8,2)$$

modulo products and modulo multiple zeta values of depth ≤ 2.

8.4 Are the exceptional elements motivic?

We say that an exceptional element e_f is *motivic* if it lies in the depth-graded motivic Lie algebra:

$$\mathsf{e}_f \in \mathfrak{dg}_4^{\mathfrak{m}} \subseteq \mathfrak{ls}_4.$$

Conjecture 3. The exceptional elements e_f are all motivic.

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Since $\mathfrak{dg}^{\mathfrak{m}}_k = \mathfrak{ls}_k$ for $k = 1, 2, 3$, to prove that an exceptional element e_f is motivic it is enough to show that, modulo commutators, it lies in the image of the map

$$d : \mathsf{S} \longrightarrow (\mathfrak{dg}^{\mathfrak{m}}_4)^{\mathrm{ab}},$$

where $\mathsf{S} \subset \Lambda^2 \mathfrak{dg}^{\mathfrak{m}}_1$ is the space of relations in depth 2, and d is the first non-trivial differential in the spectral sequence on $\mathfrak{g}^{\mathfrak{m}}$ associated to the depth filtration (§ 4.5).

The map d can be computed explicitly as follows. Choose a lift $\sigma_{2n+1} \in \mathfrak{g}^{\mathfrak{m}}$ of every generator $\bar{\sigma}_{2n+1} \in \mathfrak{dg}^{\mathfrak{m}}_1$, and decompose it according to the $\mathfrak{D}$-degree:

$$\sigma_{2n+1} = \sigma^{(1)}_{2n+1} + \sigma^{(2)}_{2n+1} + \sigma^{(3)}_{2n+1} + \cdots,$$

where $\sigma^{(i)}_{2n+1}$ is of $\mathfrak{D}$-degree i, and $\sigma^{(1)}_{2n+1} = \bar{\sigma}_{2n+1}$. Then, for any element

$$\xi = \sum_{i<j} \lambda_{i,j}\, \sigma_i \wedge \sigma_j \in \mathsf{S} = \ker(\{.\,,.\} : \Lambda^2 \mathfrak{dg}^{\mathfrak{m}}_1 \to \mathfrak{dg}^{\mathfrak{m}}_2)$$

with $\lambda_{i,j} \in \mathbb{Q}$, we have

$$d\xi = \sum_{i<j} \lambda_{i,j}(\{\sigma^{(1)}_i, \sigma^{(3)}_j\} + \{\sigma^{(2)}_i, \sigma^{(2)}_j\} + \{\sigma^{(3)}_i, \sigma^{(1)}_j\}),$$

where $\{.\,,.\} : \bigwedge^2 \mathfrak{g}^{\mathfrak{m}} \to \mathfrak{g}^{\mathfrak{m}}$ can be computed on the level of polynomial representations by exactly the same formula as the one given in § 6.

Example 8.5. The elements $\sigma_3, \sigma_5, \sigma_7, \sigma_9$ defined by the coefficients of $\zeta(3), \zeta(5), \zeta(7)$, and $\zeta(9)$ in weights 3, 5, 7, 9 in Drinfeld's associator are canonical, and we have

$$\{\sigma_3, \sigma_9\} - 3\{\sigma_5, \sigma_7\} \equiv \tfrac{691}{144}\,\mathsf{e}_{12} \mod \text{depth} \geq 5, \tag{8.8}$$

which proves that the element e_{12} is motivic. Using the depth-parity proposition (Proposition 6.4), one can show that the corresponding congruence

$$\{\sigma_3, \sigma_9\} - 3\{\sigma_5, \sigma_7\} \equiv 0 \mod 691,$$

propagates to depth 5 also. Compare with the 'key example' of [Iha02, p. 258] and the ensuing discussion. Thereafter, one checks that

$$\begin{aligned}
d\big(2\,\sigma_3 \wedge \sigma_{13} - 7\,\sigma_5 \wedge \sigma_{11} + 11\,\sigma_7 \wedge \sigma_9\big) &\equiv \tfrac{3617}{720}\mathsf{e}_{16} \pmod{\mathfrak{a}},\\
d\big(8\,\sigma_3 \wedge \sigma_{15} - 25\,\sigma_5 \wedge \sigma_{13} + 26\,\sigma_7 \wedge \sigma_{11}\big) &\equiv \tfrac{43867}{9000}\mathsf{e}_{18} \pmod{\mathfrak{a}},\\
d\big(3\,\sigma_3 \wedge \sigma_{17} - 10\,\sigma_5 \wedge \sigma_{13} + 14\,\sigma_7 \wedge \sigma_{13} - 13\,f_9 \wedge f_{11}\big) &\equiv \tfrac{174611}{35280}\mathsf{e}_{20} \pmod{\mathfrak{a}},
\end{aligned}$$

where $\mathfrak{a} = \{\mathfrak{g}^{\mathfrak{m}}, \mathfrak{g}^{\mathfrak{m}}\} + \mathfrak{D}^5\mathfrak{g}^{\mathfrak{m}}$, that is, the previous identities hold modulo commutators and modulo terms of depth 5 or more. In this manner, I have checked that the elements e_f are motivic for all f up to weight 30. In particular, it seems that the differential d is related to our map e (which is defined over $\mathbb{Z}$) up to a non-trivial isomorphism of the space of period polynomials. The numerators on the right-hand side are the numerators of $\zeta(16)\pi^{-16}, \zeta(18)\pi^{-18}$, and $\zeta(20)\pi^{-20}$. Unfortunately, it does not seem possible to construct canonical zeta elements σ_{2n+1} for $n \geq 5$ in a consistent way such that the above relations hold exactly in $\mathfrak{g}^{\mathfrak{m}}_4$ (and not modulo $\mathfrak{a}$).

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Using the theory of the unipotent fundamental group of the Tate elliptic curve, we showed in [Bro17a] how to construct canonical elements $\sigma^{(3)}_{2i+1}$ modulo depths ≥ 5, which enables one to write down the differential d explicitly. The only remaining difficulty in proving that the elements e_f are motivic is therefore to understand better the quotient $\mathfrak{ls}/\{\mathfrak{ls}, \mathfrak{ls}\}$ in depth 4. Yasuda has since shown, assuming that the e_f are motivic, how to relate the exceptional elements to the differential d using the action of Hecke operators on the space of period polynomials.

If the elements e_f can be shown to be motivic, then they provide in particular an answer to the question raised by Ihara [Iha02, end of § 4, p. 259]. The appearance of the numerators of Bernoulli numbers is related to [Iha02, Conjecture 2], and the Ihara–Takao relations [IT93], and has been studied from the Galois-theoretic perspective by Sharifi [Sha02] and McCallum and Sharifi [MS03].

9. Some properties of the elements e_f

The exceptional elements e_f satisfy many remarkable properties, only some of which will be outlined here. Of particular relevance are those properties which are *motivic*, that is, stable under the Ihara bracket.

9.1 Unevenness

For any polynomial $f \in \mathbb{Q}[x_1, \ldots, x_r]$, let

$$\pi^k_{x_i} f = \text{coefficient of } x_i^k \text{ in } f$$

and denote the projection onto the even part in x_i by

$$\pi^{\mathrm{ev}}_{x_i} f = \sum_{k \geq 0} (\pi^{2k}_i f)\, x_i^{2k}.$$

We can also write $\pi^{\mathrm{ev}}_{x_i} f = \frac{1}{2}\big(f(x_1, \ldots, x_i, \ldots, x_r) + f(x_1, \ldots, -x_i, \ldots, x_r)\big)$.

Lemma 9.1. *The elements $\mathsf{e}_f(y_0, y_1, y_2, y_3, y_4)$ are uneven:*

$$\pi^{\mathrm{ev}}_{y_0}\pi^{\mathrm{ev}}_{y_1}\pi^{\mathrm{ev}}_{y_2}\pi^{\mathrm{ev}}_{y_3}\pi^{\mathrm{ev}}_{y_4}(\mathsf{e}_f) = 0. \tag{9.1}$$

Proof. The term of the form $(y_0 - y_1) f_0(y_2 - y_3, y_4 - y_3)$ in definition (8.1) is obviously uneven since it is linear in y_0, y_1. The term $f_1(y_4 - y_3, y_2 - y_1)$ is likewise uneven because $f_1(x, y)$ is odd in x and y. The fact that e_f is uneven follows by cyclic symmetry. □

We shall see later in § 11.1 that the property of being uneven is motivic, that is, stable under the Ihara bracket, and is related to the totally odd zeta values. We conjecture that a solution to the linearized double shuffle equations is uneven if and only if it is in the Lie ideal of $\mathfrak{ls}$ generated by exceptional elements.

9.2 Sparsity

Lemma 9.2. *The elements $\mathsf{e}_f(y_0, y_1, y_2, y_3, y_4)$ are sparse:*

$$\frac{\partial^5}{\partial y_0 \partial y_1 \partial y_2 \partial y_3 \partial y_4}(\mathsf{e}_f) = 0. \tag{9.2}$$

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In other words, e_f is a linear combination of monomials which only depend on four out of five of the variables $y_0, \dots, y_4$.

Proof. Immediate from the definition. □

One can show that this property is also motivic, that is, forms an ideal under the Ihara bracket. Call an element $f \in \mathfrak{p}_r$ sparse if it is annihilated by

$$\frac{\partial^{r+1}}{\partial y_0 \dots \partial y_r}.$$

Proposition 9.3. *The sparse elements in $\bigoplus_r \mathfrak{p}_r$ form a Lie ideal.*

Proof. Let $f \in \mathfrak{p}_r$ and $g \in \mathfrak{p}_s$ where f is sparse. The Ihara bracket $\{f, g\}$ is given by (6.14) and consists of a cyclic sum over terms of the form

$$\big(f(y_0, \dots, y_r) - f(y_{r+s}, y_0, \dots, y_{r-1})\big) g(y_r, \dots, y_{r+s}),$$

to which we apply the product of $\partial/\partial y_i$ for $0 \leq i \leq r+s$. Using the chain rule with respect to $\partial/\partial y_r$ and $\partial/\partial y_{r+s}$ and invoking the sparsity of f, we obtain

$$\left(\prod_{i=0}^{r-1} \frac{\partial}{\partial y_i}\right) \big(f(y_0, \dots, y_r) - f(y_{r+s}, y_0, \dots, y_{r-1})\big) \times \left(\prod_{i=r}^{r+s} \frac{\partial}{\partial y_i}\right) g(y_r, \dots, y_{r+s}). \tag{9.3}$$

By cyclic symmetry of f, we have

$$f(y_{r+s}, y_0, \dots, y_{r-1}) = f(y_0, \dots, y_{r-1}, y_{r+s}).$$

Using the sparsity of f once more, we find that

$$\left(\prod_{i=0}^{r-1} \frac{\partial}{\partial y_i}\right) f(y_0, \dots, y_r) = \left(\prod_{i=0}^{r-1} \frac{\partial}{\partial y_i}\right) f(y_0, \dots, y_{r-1}, y_{r+s})$$

since the left-hand side is a polynomial which is annihilated by $\partial/\partial y_r$, and hence does not depend on y_r. In particular, it equals the right-hand side. It follows that the left-hand factor of (9.3) vanishes, which completes the proof. □

In fact, there are other differential equations satisfied by the e_f and one can use these equations to define various filtrations on the Lie algebras $\mathfrak{p}$ and $\mathfrak{ls}$. It would be interesting to try to prove that the degree in the exceptional elements defines a grading on the Lie subalgebra of $\bar{\mathfrak{p}}$ spanned by the x_1^{2n} and the $\bar{\mathsf{e}}_f$, as predicted by the conjectures below.

Remark 9.4. The properties of unevenness and sparsity imply that almost all the coefficients of e_f are zero. This implies that the freeness of the motivic Lie algebra (Theorem 1.1) hangs by a thread (see, for example, (8.8)).

If we define the *interior* of a polynomial $p \in \mathbb{Q}[x_1, \dots, x_r]$ to be $p^o = \pi_1^{\geq 2} \dots \pi_r^{\geq 2} p$, where $\pi_i^{\geq 2}(f) = \sum_{k \geq 2} \pi_{x_i}^k(f)\, x_i^k$, then in fact the majority of the non-trivial monomials in $\bar{\mathsf{e}}_f$ are

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determined by a single term,

$$(\bar{\mathsf{e}}_f)^o = f_1(x_4 - x_3, x_2 - x_1)^o, \tag{9.4}$$

which follows easily from the definition (8.6).

9.3 Other properties

We mention briefly some directions for further investigation. The proofs of the following facts are trivial yet sometimes lengthy applications of the definitions, basic properties of period polynomials, and the definition of $\{.\,,.\}$.

Suppose that $f^{(1)}, \dots, f^{(n)}$ are period polynomials, and let $f_1^{(i)}$ be as defined in § 8.2. Then, generalizing (8.7), we have

$$\pi^0_{n+2}\pi^0_{n+3}\dots\pi^0_{4n-1}\pi^0_{4n}\big(\bar{\mathsf{e}}_{f^{(1)}}\circ(\bar{\mathsf{e}}_{f^{(2)}}\circ\cdots(\bar{\mathsf{e}}_{f^{(n-1)}}\circ\bar{\mathsf{e}}_{f^{(n)}})\cdots)\big) = \prod_{i=1}^n f_1^{(i)}(x_i, x_{i+1}). \tag{9.5}$$

Unfortunately, some information about the polynomials f_i is lost in this equation, but one can do better by using the operators $\pi_i^{\mathrm{ev}} = \pi_{x_i}^{\mathrm{ev}}$. For example, one checks that

$$\pi_1^{\mathrm{ev}}\pi_5^{\mathrm{ev}}\pi_6^0\pi_7^0\pi_8^0\,(\bar{\mathsf{e}}_f\circ\bar{\mathsf{e}}_g) = \big(\pi_1^{\mathrm{ev}}\pi_4^0\bar{\mathsf{e}}_f(x_1,x_2,x_3,x_4)\big)\times\big(\pi_5^{\mathrm{ev}}\pi_6^0\bar{\mathsf{e}}_g(x_3,x_4,x_5,x_6)\big) \tag{9.6}$$

factorizes. Applying the operator π_3^2 to this equation gives

$$\big(\pi_3^1\pi_1^{\mathrm{ev}}\pi_4^0\bar{\mathsf{e}}_f(x_1,x_2,x_3,x_4)\big)\times\big(\pi_3^1\pi_5^{\mathrm{ev}}\pi_6^0\bar{\mathsf{e}}_g(x_3,x_4,x_5,x_6)\big)\in\mathbb{Q}[x_1,x_2]\otimes_{\mathbb{Q}}\mathbb{Q}[x_4,x_5]$$

and causes the variables to separate. Next, one checks that

$$\pi_3^1\pi_1^{\mathrm{ev}}\pi_4^0\bar{\mathsf{e}}_f(x_1,x_2,x_3,x_4) = \pi_1^{\mathrm{ev}}(\alpha(x_2-x_1)^{\deg f} + f_0(x_1, x_1+x_2))$$

for some $\alpha\in\mathbb{Q}$, and it is easy to show that the right-hand side of the previous equation is non-zero and uniquely determines the period polynomial f (using the fact that the involutions $(x_1,x_2)\mapsto(x_1,x_2-2x_1)$ and $(x_1,x_2)\mapsto(-x_1,x_2)$ generate an infinite group). Putting these facts together shows the following result.

COROLLARY 9.5. *There are no non-trivial relations between commutators* $\{\bar{\mathsf{e}}_f,\bar{\mathsf{e}}_g\}$.

Since similar factorization properties to (9.6) hold in higher depths, one might hope to prove, in a similar manner, the conjecture that the Lie subalgebra of $\mathfrak{ls}$ generated by the exceptional elements e_f is free.

10. Lie algebra structure and Broadhurst–Kreimer conjecture

10.1 Interpretation of the Broadhurst–Kreimer conjecture

In the light of the Broadhurst–Kreimer conjecture on the dimensions of the space of multiple zeta values graded by depth (1.2), and Zagier's conjecture which states that the regularized double shuffle relations generate all relations between multiple zeta values, it is natural to rephrase their conjectures, tentatively, in the Lie algebra setting as follows.

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Conjecture 4 (Strong Broadhurst–Kreimer and Zagier conjecture).

$$\begin{aligned} H_1(\mathfrak{ls}, \mathbb{Q}) &\cong \mathfrak{ls}_1 \oplus \mathsf{e}(\mathsf{S}),\\ H_2(\mathfrak{ls}, \mathbb{Q}) &\cong \mathsf{S},\\ H_i(\mathfrak{ls}, \mathbb{Q}) &= 0, \quad \text{for all } i \geq 3. \end{aligned} \tag{10.1}$$

This conjecture is the strongest possible conjecture that one could make: as we shall see below, it implies nearly all the remaining open problems concerning relations between (motivic) multiple zeta values. The numerical evidence for this conjecture is substantial [BBV10], but not sufficient to remove all reasonable doubt. More conservatively, and without reference to the double shuffle relations, one could make a weaker reformulation of the Broadhurst–Kreimer conjecture.

Conjecture 5 (Motivic version of the Broadhurst–Kreimer conjecture). The exceptional elements e_f are motivic (i.e. $\mathsf{e}(\mathsf{S}) \subset \mathfrak{dg}^{\mathfrak{m}}$), and

$$\begin{aligned} H_1(\mathfrak{dg}^{\mathfrak{m}}, \mathbb{Q}) &\cong \mathfrak{dg}^{\mathfrak{m}}_1 \oplus \mathsf{e}(\mathsf{S}),\\ H_2(\mathfrak{dg}^{\mathfrak{m}}, \mathbb{Q}) &\cong \mathsf{S},\\ H_i(\mathfrak{dg}^{\mathfrak{m}}, \mathbb{Q}) &= 0, \quad \text{for all } i \geq 3. \end{aligned} \tag{10.2}$$

Since the conjectural generators are totally explicit, it is possible to verify the independence of Lie brackets in the reduced polynomial representation $\bar{\rho}(\mathfrak{g}^{\mathfrak{m}})$ simply by computing the coefficients of a small number of monomials. In this way, it should be possible to verify (10.2) to much higher weights and depths than is presently known. Note that the Broadhurst–Kreimer conjecture could fail if there existed non-trivial relations between commutators involving several exceptional elements e_f. These would necessarily have weight and depth far beyond the range of present computations.

10.2 Enumeration of dimensions

Let $\mathfrak{h}$ be a Lie algebra over a field k, and let $\mathcal{U}\mathfrak{h}$ be its universal enveloping algebra. The homology groups $H_i(\mathfrak{h}; k)$ of $\mathfrak{h}$ are defined to be the homology of the following complex:

$$\cdots \longrightarrow \Lambda^3\mathfrak{h} \longrightarrow \Lambda^2\mathfrak{h} \longrightarrow \mathfrak{h} \longrightarrow 0. \tag{10.3}$$

Suppose that $\mathfrak{h}$ is bigraded, and finite-dimensional in each bigraded piece. Then $\Lambda^i\mathfrak{h}, \mathcal{U}\mathfrak{h}, H_i(\mathfrak{h})$ inherit a bigrading. For any bigraded k-module $M_{\bullet,\bullet}$, which is finite-dimensional in every bidegree, define its Poincaré–Hilbert series by

$$\mathcal{X}_M(s,t) = \sum_{m,n\geq 0} \dim_k(M_{m,n}) s^m t^n.$$

Similarly, for a family of such bigraded k-modules M^l, with $l \geq 0$, let us write

$$\mathcal{X}_{M^\bullet}(r,s,t) = \sum_{l,m,n\geq 0} \dim_k(M^l_{m,n}) r^l s^m t^n.$$

The following proposition follows from standard homological algebra.

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Proposition 10.1. *With the above assumptions, the Poincaré series of $\mathcal{U}\mathfrak{h}$ and the homology of $\mathfrak{h}$ are related by the equation*

$$\mathcal{X}_{\mathcal{U}\mathfrak{h}}(s,t) = \frac{1}{\mathcal{X}_{H_\bullet(\mathfrak{h})}(-1,s,t)}. \tag{10.4}$$

Proof. Let $\varepsilon : \mathcal{U}\mathfrak{h} \to k$ be the augmentation map. Recall that the Chevalley–Eilenberg complex [Wei94, § 7.7] is exact in all degrees:

$$\cdots \longrightarrow \mathcal{U}\mathfrak{h} \otimes_k \Lambda^2 \mathfrak{h} \longrightarrow \mathcal{U}\mathfrak{h} \otimes_k \mathfrak{h} \longrightarrow \mathcal{U}\mathfrak{h} \xrightarrow{\varepsilon} k \longrightarrow 0. \tag{10.5}$$

It therefore defines a resolution of k. Viewing k as a $\mathcal{U}\mathfrak{h}$-module via ε and applying the functor $M \mapsto k \otimes_{\mathcal{U}\mathfrak{h}} M$ to (10.5) gives a complex whose truncation is exactly (10.3).

Writing $\Lambda^1\mathfrak{h} = \mathfrak{h}$, and $\Lambda^0\mathfrak{h} = k$, the exactness of (10.5) yields

$$1 = \sum_{l\geq 0} (-1)^l \mathcal{X}_{\mathcal{U}\mathfrak{h}}(s,t)\mathcal{X}_{\Lambda^l\mathfrak{h}}(s,t) = \mathcal{X}_{\mathcal{U}\mathfrak{h}}(s,t)\mathcal{X}_{\Lambda^\bullet\mathfrak{h}}(-1,s,t),$$

since this is nothing other than the bigraded Euler characteristic. Since (10.3) computes the homology of $\mathfrak{h}$, we deduce similarly that

$$\mathcal{X}_{\Lambda^\bullet\mathfrak{h}}(-1,s,t) = \mathcal{X}_{H_\bullet(\mathfrak{h})}(-1,s,t)$$

which implies formula (10.4). □

10.3 Corollaries of Conjectures 4 and 5

Let us first apply Proposition 10.1 to the algebra $\mathfrak{ls}$, bigraded by weight and depth.

Lemma 10.2. *Conjecture 4 implies that*

$$\mathcal{X}_{\mathcal{U}\mathfrak{ls}}(s,t) = \frac{1}{1 - \mathbb{O}(s)\, t + \mathbb{S}(s)\, t^2 - \mathbb{S}(s)\, t^4}. \tag{10.6}$$

If we identify $\mathfrak{ls}_d$ via the isomorphism $\bar{\rho}$ with the space of polynomials $\mathbb{D}_d$ satisfying the linearized double shuffle relations, we obtain the conjecture stated in [IKZ06, Appendix].

Proof. Assuming Conjecture 4, we have

$$\mathcal{X}_{H_1(\mathfrak{ls})}(s,t) = \mathbb{O}(s)\, t + \mathbb{S}(s)\, t^4,$$
$$\mathcal{X}_{H_2(\mathfrak{ls})}(s,t) = \mathbb{S}(s)\, t^2,$$

where $\mathbb{O}$ and $\mathbb{S}$ were defined in (1.3). Apply (10.4) to conclude. □

Proposition 10.3. *Conjecture 4 is equivalent to Conjecture 5, together with $\mathfrak{dg}^{\mathfrak{m}} = \mathfrak{ls}$.*

Proof. The inclusion $\mathfrak{dg}^{\mathfrak{m}} \subset \mathfrak{ls}$ implies that, for all weights N and depths d,

$$\dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{g}^{\mathfrak{m}})_{N,d} \leq \dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{ls})_{N,d}. \tag{10.7}$$

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This uses the fact that $\mathrm{gr}_{\mathfrak{D}}\mathcal{U}\mathfrak{g}^{\mathfrak{m}} \cong \mathcal{U}\mathfrak{dg}^{\mathfrak{m}}$, which follows from the Poincaré–Birkoff–Witt theorem. Now we know from Theorem 1.1 that

$$\frac{1}{1-\mathbb{O}(s)} = \sum_{N\geq 0}\bigg(\sum_{d\geq 0}\dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{g}^{\mathfrak{m}})_{N,d}\bigg)s^N.$$

If conjecture 4 holds then, specializing (10.6) to $t=1$, we obtain

$$\frac{1}{1-\mathbb{O}(s)} = \sum_{N\geq 0}\bigg(\sum_{d\geq 0}\dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{ls})_{N,d}\bigg)s^N,$$

and therefore, for all N,

$$\sum_{d\geq 0}\dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{g}^{\mathfrak{m}})_{N,d} = \sum_{d\geq 0}\dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{ls})_{N,d}.$$

Since the dimensions in (10.7) are non-negative, this implies equality in (10.7), and so $\mathrm{gr}_{\mathfrak{D}}\mathcal{U}\mathfrak{g}^{\mathfrak{m}} \cong \mathcal{U}\mathfrak{dg}^{\mathfrak{m}} = \mathcal{U}\mathfrak{ls}$ and hence $\mathfrak{dg}^{\mathfrak{m}} = \mathfrak{ls}$. Replacing $\mathfrak{dg}^{\mathfrak{m}}$ with $\mathfrak{ls}$ in Conjecture 4 gives the statement of Conjecture 5, and proves the first direction of the implication. The converse is obvious. □

The conjecture $\mathfrak{dg}^{\mathfrak{m}} = \mathfrak{ls}$ implies that $\mathfrak{g}^{\mathfrak{m}} = \mathfrak{dm}_0(\mathbb{Q})$, which is the statement that all relations between motivic multiple zeta values are generated by the regularized double shuffle relations (which is equivalent to a conjecture of Zagier's). By Furusho's theorem [Fur11], it would in turn imply Drinfeld's conjecture that $\mathfrak{grt}$ is free with one generator in every odd degree ≤ -3 (which is in turn equivalent, in the light of Theorem 1.1, to the statement that all relations between (motivic) multiple zeta values are generated by the associator relations.)

Corollary 10.4. *Conjecture 5 implies a Broadhurst–Kreimer conjecture for motivic multiple zeta values. More precisely, Conjecture 5 implies that*

$$\sum_{N,d\geq 0}(\dim_{\mathbb{Q}}\mathrm{gr}_d^{\mathfrak{D}}\mathcal{H}_N)\, s^N t^d = \frac{1+\mathbb{E}(s)t}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2-\mathbb{S}(s)t^4}, \tag{10.8}$$

where $\mathcal{H}_N$ is the $\mathbb{Q}$-vector space generated by motivic multiple zeta values of weight N.

Proof. Apply Proposition 10.1 to $\mathfrak{dg}^{\mathfrak{m}}$. Then Conjecture 5 implies via (10.4) that

$$\sum_{N,d\geq 0}(\dim_{\mathbb{Q}}\mathrm{gr}^d_{\mathfrak{D}}\mathcal{U}\mathfrak{g}^{\mathfrak{m}}_N)s^N t^d = \frac{1}{1-\mathbb{O}(s)\,t+\mathbb{S}(s)\,t^2-\mathbb{S}(s)\,t^4}. \tag{10.9}$$

Equation (10.8) follows from (4.3), which states that

$$\mathrm{gr}^{\mathfrak{D}}\mathcal{H} \cong \big(\mathrm{gr}^{\mathfrak{D}}\mathcal{A}\big)\otimes_{\mathbb{Q}}\big(\mathrm{gr}^{\mathfrak{D}}\mathbb{Q}[\zeta^{\mathfrak{m}}(2)]\big).$$

The statement follows from $\mathrm{gr}^{\mathfrak{D}}\mathcal{A} \cong (\mathrm{gr}_{\mathfrak{D}}\mathcal{U}\mathfrak{g}^{\mathfrak{m}})^{\vee}$ (see § 4.2) and the fact that $1+\mathbb{E}(s)t$ is the Poincaré series for the bigraded algebra

$$\mathrm{gr}^{\mathfrak{D}}\mathbb{Q}[\zeta^{\mathfrak{m}}(2)] = \mathbb{Q}\oplus\bigoplus_{n\geq 1}\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n)\mathbb{Q}$$

using a corollary [Bro12] of the motivic version of Euler's theorem: $\mathbb{Q}\zeta^{\mathfrak{m}}(2n) = \mathbb{Q}\zeta^{\mathfrak{m}}(2)^n$. □

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11. Totally odd multiple zeta values

Let $\mathcal{H}^{\mathrm{odd}} \subset \mathcal{H}$ denote the vector subspace generated by the elements

$$\zeta^{\mathfrak{m}}(2n_1+1,\dots,2n_r+1), \tag{11.1}$$

where $n_1,\dots,n_r$ are integers ≥ 1. Then $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{\mathrm{odd}} \subset \mathrm{gr}^{\mathfrak{D}}\mathcal{H}$ is the vector subspace spanned by the depth-graded versions $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n_1+1,\dots,2n_r+1)$ of (11.1). It is clear from the linearized stuffle product formula that $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{\mathrm{odd}}$ is an algebra, indeed, it is a quotient of the shuffle algebra

$$\big(\mathbb{Q}\langle \mathsf{3},\mathsf{5},\mathsf{7},\dots,\rangle, ш\big)$$

with exactly one generator $\mathsf{2n+1}$ in each degree $2n+1$, for $n\geq 1$. Let $\mathcal{A}^{\mathrm{odd}}$ denote $\mathcal{H}^{\mathrm{odd}}$ modulo the ideal generated by $\zeta^{\mathfrak{m}}(2)$, and let $\mathrm{gr}^{\mathfrak{D}}\mathcal{A}^{\mathrm{odd}}$ denote $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{\mathrm{odd}}$ modulo the ideal generated by $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2)$.

Proposition 11.1. *The space $\mathcal{H}^{\mathrm{odd}}$ is almost stable under the motivic coaction:*

$$\Delta^{\mathcal{M}}(\mathfrak{D}_r\mathcal{H}^{\mathrm{odd}}) \subseteq \mathcal{A}\otimes\mathfrak{D}_r\mathcal{H}^{\mathrm{odd}} + \mathcal{A}\otimes\mathfrak{D}_{r-2}\mathcal{H}.$$

Furthermore, the group $\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$ acts trivially on the associated graded $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{\mathrm{odd}}$.

Proof. By the remarks at the end of § 3.1, it suffices to compute the infinitesimal coaction (3.3) in odd degrees only. Therefore apply the operator D_{2s+1} to the element

$$I^{\mathfrak{m}}(0;1,\underbrace{0,\dots,0}_{2n_1},1,\underbrace{0,\dots,0}_{2n_2},\dots,1,\underbrace{0,\dots,0}_{2n_r};1).$$

We use the terminology 'subsequence' to denote a term which occurs on the left-hand side of (3.3), and 'quotient sequence' to denote a term which occurs on the right. Every subsequence with two or more 1's gives rise to a quotient sequence of depth $\leq r-2$. Every subsequence of depth exactly 1 and of odd length is either of the form

$$I^{\mathfrak{m}}(0;\underbrace{0,\dots,0}_{\text{odd}},1,\underbrace{0,\dots,0}_{\text{odd}};1) \quad \text{or} \quad I^{\mathfrak{m}}(1;\underbrace{0,\dots,0}_{\text{odd}},1,\underbrace{0,\dots,0}_{\text{odd}};0)$$

(which cannot occur since every pair of successive 1's in the original sequence are separated by an even number of 0's), or of the form

$$I^{\mathfrak{m}}(0;\underbrace{0,\dots,0}_{\text{even}},1,\underbrace{0,\dots,0}_{\text{even}};1) \quad \text{or} \quad I^{\mathfrak{m}}(1;\underbrace{0,\dots,0}_{\text{even}},1,\underbrace{0,\dots,0}_{\text{even}};0).$$

In this case, the quotient sequence has the property that every pair of successive 1's are separated by an even number of 0's, which defines an element of $\mathcal{H}^{\mathrm{odd}}$. In the case when the subsequence has no 1's, the left-hand side of (3.3) is zero and the action is trivial, which proves the last statement. $\square$

It follows immediately from the proposition that the action of the graded Lie algebra $\mathrm{Lie}\,\mathcal{U}_{\mathcal{MT}(\mathbb{Z})}$ on the two-step quotients $\mathfrak{D}_r\mathcal{H}^{\mathrm{odd}}/\mathfrak{D}_{r-2}\mathcal{H}^{\mathrm{odd}}$ factors through its abelianization $(\mathrm{Lie}\,\mathcal{U}_{\mathcal{MT}(\mathbb{Z})})^{\mathrm{ab}}$, which has canonical generators in every odd degree $2r+1$, for $r\geq 1$.

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Thus for every integer $n \geq 1$, there is a well-defined derivation

$$\partial_{2n+1} : \mathrm{gr}_r^{\mathfrak{D}} \mathcal{H}^{\mathrm{odd}} \longrightarrow \mathrm{gr}_{r-1}^{\mathfrak{D}} \mathcal{H}^{\mathrm{odd}},$$

which corresponds to the action of the canonical generator $\sigma_{2n+1} \in (\mathrm{Lie}\,\mathcal{U}_{\mathcal{MT}(\mathbb{Z})})^{\mathrm{ab}}$. If $m_1 + \cdots + m_r = n_1 + \cdots + n_r$ are integers ≥ 1, then we obtain numbers

$$c_{\left(\substack{m_1 \ldots m_r \\ n_1 \ldots n_r}\right)} = \partial_{2m_1+1} \ldots \partial_{2m_{r-1}+1} \partial_{2m_r+1}\, \zeta_{\mathfrak{D}}^{\mathfrak{m}}(2n_1+1, \ldots, 2n_r+1) \in \mathbb{Z}$$

where, by duality,

$$c_{\left(\substack{m_1 \ldots m_r \\ n_1 \ldots n_r}\right)} = \text{coefficient of } x_1^{2n_1} \ldots x_r^{2n_r} \quad \text{in } x_1^{2m_r} \,\underline{\circ}\, (x_2^{2m_{r-1}} \,\underline{\circ}\, (\cdots (x_{r-1}^{2m_2} \,\underline{\circ}\, x_r^{2m_1}) \cdots).$$

Recall that the action $\underline{\circ}$ is given by the formula

$$\mathbb{Q}[x_1^2] \otimes_{\mathbb{Q}} \mathbb{Q}[x_1, \ldots, x_{r-1}] \longrightarrow \mathbb{Q}[x_1, \ldots, x_r]$$
$$x_1^{2n} \,\underline{\circ}\, g(x_1, \ldots, x_{r-1}) = \sum_{i=1}^{r} \big((x_i - x_{i-1})^{2n} - (x_i - x_{i+1})^{2n} \big) g(x_1, \ldots, \widehat{x_i}, \ldots, x_r),$$

where $x_0 = 0$ and $x_{r+1} = x_r$ (i.e. the term $(x_r - x_{r+1})^{2n}$ is discarded). Note that $\underline{\circ}$ coincides with $\circ$ here by Proposition 2.2 since x_1^{2n} lies in the image of $\mathfrak{g}^{\mathfrak{m}}$.

If $S_{N,r}$ denotes the set of compositions of an integer N as a sum of r positive integers, let $C_{N,r}$ denote the $|S_{N,r}| \times |S_{N,r}|$ square matrix whose entries are the integers

$$(C_{N,r})_{i,j} = c_{\left(\substack{s_i \\ s_j}\right)}, \quad s_i, s_j \in S_{N,r}. \tag{11.2}$$

11.1 Enumeration of totally odd depth-graded multiple zeta values

Definition 11.2. We say that a polynomial $f \in \mathbb{Q}[y_0, y_1, \ldots, y_r]$ is *uneven* if the coefficient of $y_0^{2n_0} \ldots y_r^{2n_r}$ in f vanishes for all $n_0, \ldots, n_r \geq 0$.

Recall from (9.1) that the exceptional elements $e_f \in \mathfrak{ls}$ are uneven. The following proposition is a kind of dual to the previous one.

Proposition 11.3. *The set of uneven elements in $\mathfrak{ls}$ is an ideal for the Ihara bracket.*

Proof. Let $f, g \in \rho(\mathfrak{ls})$ such that f is uneven. It suffices to show that $\{f, g\}$ is uneven. By the parity result (Proposition 6.4), we know that f and g are of even degree. It follows from (6.3) that $\{f, g\}$ is a linear combination of terms of the form

$$f(y_\alpha) g(y_\beta),$$

where α, β are sets of indices with $|\alpha \cap \beta| = 1$. Since the polynomial f is homogeneous of even degree, it follows that the coefficient of $y_0^{2n_0} \ldots y_N^{2n_N}$ in $\{f, g\}$ is a linear combination of the coefficients of totally even monomials in f, which all vanish. In more detail, let us consider two sets of indices with $\alpha \cap \beta = \{\gamma\}$, and the corresponding monomials which occur in f, g respectively:

$$c_\alpha^f \prod_{a \in \alpha} y_a^{m_a} \quad \text{and} \quad c_\beta^g \prod_{b \in \beta} y_b^{n_a},$$

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where $c^f_\alpha, c^g_\beta \in \mathbb{Q}$. A monomial in $\{f,g\}$ is of the form

$$c^f_\alpha c^g_\beta\, y_\gamma^{m_\gamma+n_\gamma} \prod_{a\in\alpha\backslash\{\gamma\}} y_a^{m_a} \prod_{b\in\beta\backslash\{\gamma\}} y_b^{n_b}.$$

Suppose that $m_\gamma+n_\gamma$ and all m_a, n_b are even for $a\in\alpha\backslash\{\gamma\}$ and $b\in\beta\backslash\{\gamma\}$. If m_γ is odd, then $c^f_\alpha=0$ since f is of even degree by Proposition 6.4. In the case when m_γ is even, $c^f_\alpha=0$ since f is uneven. Therefore $\{f,g\}$ is uneven. □

Corollary 11.4. *The Lie ideal in $\mathfrak{ls}$ generated by the exceptional elements is orthogonal to (i.e. annihilated by)* $\mathrm{gr}^{\mathfrak{D}}\mathcal{A}^{\mathrm{odd}}$.

Proof. The elements e_f are uneven. □

In the light of Conjecture 5 it is therefore natural to expect that $\mathrm{gr}^{\mathfrak{D}}\mathcal{A}^{\mathrm{odd}}$ is dual to $\mathfrak{g}^{\mathrm{odd}}$, which suggests the following conjecture.

Conjecture 6 ('Uneven' part of motivic Broadhurst–Kreimer conjecture).

$$\sum_{N\geq 0, d\geq 0} (\dim_{\mathbb{Q}} \mathrm{gr}^{\mathfrak{D}}_d \mathcal{A}^{\mathrm{odd}}_N) s^N t^d = \frac{1}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2}. \tag{11.3}$$

Since the action of the operators ∂_{2n+1} on the totally odd depth-graded motivic multiple zeta values can be computed explicitly in terms of binomial coefficients, one can hope to prove a version of this conjecture by elementary methods. Indeed, assuming Conjecture 5, the left-hand side of (11.3) is the generating series

$$\sum_{N\geq 0, d\geq 0} \mathrm{rank}(C_{N,d})\, s^N t^d,$$

where $C_{N,r}$ are the matrices of binomial coefficients defined in (11.2). Therefore, one is led to conjecture that this generating series also coincides with the right-hand side of (11.3). I have verified this up to weight 30.

Standard transcendence conjectures for multiple zeta values would then have it that if $\mathcal{Z}^{\mathrm{odd}}_{N,d}$ denotes the space of totally odd depth-graded multiple zeta values modulo $\zeta(2)$, of weight N and depth d, then we obtain the new conjecture

$$\sum_{N\geq 0, d\geq 0} \big(\dim_{\mathbb{Q}} \mathcal{Z}^{\mathrm{odd}}_{N,d}\big) s^N t^d = \frac{1}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2}. \tag{11.4}$$

Remark 11.5. These conjectures measure the relations between totally odd (motivic) multiple zeta values *modulo all (motivic) multiple zeta values of lower depth*, not just modulo totally odd (motivic) multiple zeta values of lower depth (in other words, $\mathcal{Z}^{\mathrm{odd}}_{N,d}$ denotes the span of the totally odd zetas in the space of depth- graded multiple zeta values, and not the depth-graded of the space of totally odd multiple zeta values).

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