DEPTH-GRADED MOTIVIC MULTIPLE ZETA VALUES

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Abstract. We study the depth filtration on motivic multiple zeta values, and its relation to modular forms. Using period polynomials for cusp forms for $PSL_2(\mathbb{Z})$, we construct an explicit Lie algebra of solutions to the linearized double shuffle equations over the integers, which conjecturally describes all relations between depth-graded motivic multiple zeta values (modulo $\zeta(2)$). The Broadhurst-Kreimer conjecture is recast as a statement about the homology of this Lie algebra.

To Pierre Cartier, with great admiration, on the occasion of his 80^{th} *birthday.*

1. Introduction

1.1. **Motivic multiple zeta values and the depth filtration.** Multiple zeta values are defined for integers $n_1, \ldots, n_r \geq 1$ and $n_r \geq 2$ by

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

Their weight is the quantity $n_1 + \ldots + n_r$, and their depth is the number of indices r. Since the standard transcendence conjectures for multiple zeta values are inaccessible, one can replace the study of multiple zeta values with motivic multiple zeta values

$$\zeta^{\mathfrak{m}}(n_1, \ldots, n_r) \tag{1.1}$$

which are elements of a certain algebra $\mathcal{H} = \bigoplus_N \mathcal{H}_N$ over $\mathbb{Q}$, which is graded for the weight. The period homomorphism $per : \mathcal{H} \to \mathbb{R}$ maps the element $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$ to the real number $\zeta(n_1, \ldots, n_r)$. The algebra $\mathcal{H}$ carries an action of the motivic Galois group of the category of mixed Tate motives over $\mathbb{Z}$, and its structure is known [1, 6].

Theorem 1.1. *The Hoffman motivic multiple zeta values*

$$\zeta^{\mathfrak{m}}(n_1, \ldots, n_r) \quad \text{where } n_i = 2 \text{ or } 3 \tag{1.2}$$

are a basis for $\mathcal{H}$.

In particular, the Poincaré series for motivic multiple zeta values satisfies

$$\sum_{N \geq 0} \dim_{\mathbb{Q}} (\mathcal{H}_N) s^N = \frac{1}{1 - s^2 - s^3} \ , \tag{1.3}$$

giving an upper bound for the dimension of the space of multiple zeta values of fixed weight (first proved by Terasoma, and Goncharov). Since the depth filtration is motivic [8, 7], the algebra $\mathcal{H}$ also inherits the depth filtration $\mathfrak{D}$, and one can define its associated graded algebra $\mathrm{gr}^{\mathfrak{D}} \mathcal{H}$. The depth-graded motivic multiple zeta value

$$\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r) \in \mathrm{gr}^{\mathfrak{D}}_r \mathcal{H} \tag{1.4}$$

is given by the class of (1.1) modulo elements of lower depth. Note that the depth-graded Hoffman elements $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r)$, where $n_i = 2$ or 3, lie in depths $\lceil \frac{n}{3} \rceil \leq r \leq \lfloor \frac{n}{2} \rfloor$, and are almost all zero. It follows that theorem 1.1 tells us next to nothing about the structure of depth-graded multiple zeta values.

Based on extensive computer calculations (see [5] for the current state of affairs) and some inspired guesswork, Broadhurst and Kreimer made a conjecture on the Poincaré series for the number of multiple zeta values graded for the depth [3]. Transposing this conjecture to depth-graded motivic multiple zeta values, one obtains:

Conjecture 1. (Broadhurst-Kreimer)

$$\sum_{N,d\geq 0} \dim_{\mathbb{Q}} (\mathrm{gr}^{\mathfrak{D}}_d \mathcal{H}_N)\, s^N t^d = \frac{1+\mathbb{E}(s)t}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2-\mathbb{S}(s)t^4} \ , \tag{1.5}$$

where, using the notation from ([13], appendix),

$$\mathbb{E}(s) = \frac{s^2}{1-s^2} \quad , \quad \mathbb{O}(s) = \frac{s^3}{1-s^2} \quad , \quad \mathbb{S}(s) = \frac{s^{12}}{(1-s^4)(1-s^6)} \ . \tag{1.6}$$

Note that equation (1.5) specializes to (1.3) on setting t equal to 1. 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. The interpretation of $\mathbb{S}(s)$ as the generating series for the dimensions of the space of cusp forms for the full modular group $PSL_2(\mathbb{Z})$ is due to Zagier. It follows from work of Zagier, and Goncharov, that formula (1.5) has been confirmed in depths 2 and 3 (i.e., modulo t^4).

Indeed, the relation between the coefficient $\mathbb{S}(s)$ of t^2 in the denominator of (1.5) and multiple zeta values of depth 2 is now well-understood by the work of Gangl, Kaneko and Zagier [14]. They exhibited an infinite family of exotic relations between multiple zeta values of depth 2, associated to each even period polynomial for cusp forms on $PSL_2(\mathbb{Z})$. The smallest such relation occurs in weight twelve:

$$28\,\zeta(3,9) + 150\,\zeta(5,7) + 168\,\zeta(7,5) = \frac{5197}{691}\zeta(12) \ . \tag{1.7}$$

The aim of these notes is to study the Broadhurst-Kreimer conjecture from the motivic point of view, and to try to explain the relationship between modular forms and depth-graded motivic multiple zeta values in all depths.

1.2. **The dual Lie algebra.** Throughout, let $\mathfrak{g}$ denote the graded Lie algebra over $\mathbb{Q}$ freely generated by two elements e_0, e_1 of degree -1 (it is the graded Lie algebra of the de Rham fundamental group of the projective line minus three points). Its universal enveloping algebra is the tensor algebra:

$$\mathcal{U}\mathfrak{g} = \bigoplus_{n\geq 0} (\mathbb{Q}\, e_0 \oplus \mathbb{Q}\, e_1)^{\otimes n} \ , \tag{1.8}$$

where the multiplication is given by the concatenation product, and its coproduct is the unique coproduct for which e_0 and e_1 are primitive.

Consider the following motivic version of Drinfel'd's associator

$$\Phi^{\mathfrak{m}} = \sum_w w\, \zeta^{\mathfrak{m}}(w) \quad \in \quad \mathcal{H}\langle\langle e_0, e_1 \rangle\rangle \tag{1.9}$$

where the sum is over all words w in e_0, e_1, and $\zeta^{\mathfrak{m}}(w)$ is the (shuffle-regularized) motivic multiple zeta value, which is uniquely determined by

$$\zeta^{\mathfrak{m}}(e_1 e_0^{n_1-1} \ldots e_1 e_0^{n_r-1}) = \zeta^{\mathfrak{m}}(n_1, \ldots, n_r) \ ,$$

for $n_1, \ldots, n_r$ as above, the identities $\zeta^{\mathfrak{m}}(e_1) = \zeta^{\mathfrak{m}}(e_0) = 0$, and the fact that its linear extension is a homomorphism for the shuffle product: $\zeta^{\mathfrak{m}}(w \,ш\, w') = \zeta^{\mathfrak{m}}(w)\zeta^{\mathfrak{m}}(w')$.[1]

[1] Strictly speaking, the argument w of $\zeta^{\mathfrak{m}}(w)$ should be viewed in the dual alphabet $\{e^0, e^1\}$ where $\langle e^a, e_b \rangle = \delta_{a,b}$. For the purposes of this introduction, (and also in §5) we shall ignore this distinction.

The element $\Phi^{\mathfrak{m}}$ defines a map from the graded dual of $\mathcal{H}$ to $\mathcal{U}\mathfrak{g}$

$$\bigoplus_{n\geq 0} \mathcal{H}_n^{\vee} \longrightarrow \mathcal{U}\mathfrak{g}\ . \tag{1.10}$$

The problem of describing the image of this map is equivalent to describing all relations between motivic multiple zeta values, and is very far from being solved, even conjecturally. To simplify this problem, let $\mathcal{L}$ denote the largest quotient of $\mathcal{H}$ in which $\zeta^{\mathfrak{m}}(2)$, and all non-trivial products are zero. It is graded by the weight.

Definition 1.2. The set of motivic elements $\mathfrak{g}^{\mathfrak{m}}$ is the image of $\bigoplus_{n\geq 0} \mathcal{L}_n^{\vee}$ in $\mathcal{U}\mathfrak{g}$.

The action of the motivic Galois group on the motivic multiple zeta values makes $\mathcal{L}$ into a Lie coalgebra, and hence $\mathfrak{g}^{\mathfrak{m}}$ into a Lie algebra for the Ihara bracket, which is denoted by $\{.,.\}$. The following theorem is a consequence of theorem 1.1, together with the structure of the category of mixed Tate motives over $\mathbb{Z}$.

Theorem 1.3. *The graded 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 $i \geq 1$.*

Note that the classes $[\sigma_{2i+1}]$ in $(\mathfrak{g}^{\mathfrak{m}})^{ab}$ are canonical, the elements σ_{2i+1} are not. Since $H_1(\mathfrak{g}^{\mathfrak{m}};\mathbb{Q}) = (\mathfrak{g}^{\mathfrak{m}})^{ab}$, one way to rephrase the previous theorem is to say that

$$\begin{aligned} H_1(\mathfrak{g}^{\mathfrak{m}};\mathbb{Q}) &\cong \bigoplus_{i\geq 1} [\sigma_{2i+1}]\mathbb{Q} \\ H_i(\mathfrak{g}^{\mathfrak{m}};\mathbb{Q}) &= 0 \quad \text{for} \quad i \geq 2\ . \end{aligned} \tag{1.11}$$

In principle, we could use the known bases of $\mathcal{H}$ to define 'canonical' generators of $\mathfrak{g}^{\mathfrak{m}}$ but very little is known about the coefficients of such generators[2]. Thus the problem of describing the image of (1.10) above now becomes the following:

Problem 1. Write down explicit generators for $\mathfrak{g}^{\mathfrak{m}}$ as elements of $\mathcal{U}\mathfrak{g}$.

A solution to this problem would encode all relations between motivic multiple zeta values (modulo $\zeta^{\mathfrak{m}}(2)$), and would give an exact algorithm, building on [2], to write multiple zeta values in terms of any chosen basis modulo $\zeta^{\mathfrak{m}}(2)$; bound the heights of the coefficients, and so on. Note that we do not even have an explicit conjectural description of the generators of $\mathfrak{g}^{\mathfrak{m}}$. In these notes, we shall propose, granting conjecture 1.5, a solution to the depth-graded version of problem 1.

1.3. **Depth-graded Lie algebra.** The depth filtration $\mathfrak{D}$ is the decreasing filtration on $\mathcal{U}\mathfrak{g}$ such that $\mathfrak{D}^r\mathcal{U}\mathfrak{g}$ is spanned by the set of words w in e_0, e_1 which have at least r occurrences of the letter e_1. One verifies that the Ihara bracket is homogeneous with respect to the $\mathfrak{D}$-degree. Define the Lie algebra of depth-graded motivic elements $\mathfrak{dg}^{\mathfrak{m}} \subset \mathcal{U}\mathfrak{g}$ to be the associated bigraded Lie algebra

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

It is the Lie algebra dual to the space of depth-graded motivic multiple zeta values $\zeta_{\mathfrak{D}}(w)$, for $w \in \{e_0, e_1\}^{\times}$, modulo non-trivial products, and modulo $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2)$.

In depth one, there are canonical elements, for each $i \geq 1$:

$$\overline{\sigma}_{2i+1} = (-1)^i (ad\, e_0)^{2i}(e_1) \in \mathfrak{dg}^{\mathfrak{m}}_1\ . \tag{1.12}$$

Furthermore it is known [19, 9, 14] that an expression of weight $2n$ and depth two:

$$\sum_{i<j} \lambda_{i,j} \{\overline{\sigma}_{2i+1}, \overline{\sigma}_{2j+1}\} \in \mathfrak{dg}^{\mathfrak{m}}_2 \tag{1.13}$$

[2] One could take, for instance, the polynomial system of generators for $\mathcal{H}$ given in [1], theorem 8.1, and define σ_{2i+1} to be the coefficient of $\zeta^{\mathfrak{m}}(3, 2, \ldots, 2)$, with $i-1$ two's, in $\Phi^{\mathfrak{m}}$.

vanishes if and only if the λ_{ij} are the coefficients of a period polynomial:

$$P(X,Y) = \sum_{i,j} (\lambda_{ij} - \lambda_{ji}) X^{2i} Y^{2j} \in \mathsf{S}_{2n} \ ,$$

where $\mathsf{S}_{2n} \subset \mathbb{Q}[X,Y]$ is the vector space of antisymmetric homogeneous polynomials $P(X,Y)$ of degree $2n-2$, which are divisible by Y, satisfy $P(\pm X, \pm Y) = P(X,Y)$ and

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

The smallest relation (1.13) occurs in weight 12 and was found by Ihara.

Since the Lie subalgebra of $\mathfrak{dg}^{\mathfrak{m}}$ generated by the elements $\overline{\sigma}_{2i+1}$ is not free, it must be the case that $\mathfrak{dg}^{\mathfrak{m}}$ has exceptional generators in higher depth in order to square with theorem 1.3. The Broadhurst-Kreimer conjecture suggests that such generators exist in depth 4, and the obvious way to construct them would be to consider the first non-trivial differential in the spectral sequence on $\mathfrak{g}^{\mathfrak{m}}$ associated to the depth filtration, which gives a map $d : H_2(\mathfrak{dg}^{\mathfrak{m}};\mathbb{Q}) \to H_1(\mathfrak{dg}^{\mathfrak{m}};\mathbb{Q})$, and in particular a linear map

$$d : \mathsf{S}_{2n} \longrightarrow (\mathfrak{dg}^{\mathfrak{m}}_4)^{ab} \ . \qquad (1.14)$$

Computing (1.14) is complicated by the fact that the depth 3 part of (some choice of) generators σ_{2i+1} is not known, and have complicated denominators (§8.3).

Surprisingly, there is a way to write down candidate generators over $\mathbb{Z}$ explicitly in $\mathfrak{dg}^{\mathfrak{m}}$ in depth 4 (rather than its abelianization) using modular forms. See definition 8.1. For this, we use the known relations satisfied by multiple zeta values.

1.4. **Linearized double shuffle relations.** The linearized double shuffle relations for multiple zeta values were studied in [13], §8. These consist of two sets of relations: the standard shuffle relations for multiple zeta values (which are already homogeneous for the $\mathfrak{D}$-grading), and the terms of highest $\mathfrak{D}$-degree in the second shuffle, or 'stuffle' relations. For example, the terms of highest $\mathfrak{D}$-degree in the relation

$$\zeta^{\mathfrak{m}}(m)\zeta^{\mathfrak{m}}(n) = \zeta^{\mathfrak{m}}(m,n) + \zeta^{\mathfrak{m}}(n,m) + \zeta^{\mathfrak{m}}(m+n) \qquad \text{for all } m,n \geq 2$$

taken modulo products, leads to the linearized stuffle relation

$$\zeta^{\mathfrak{m}}_{\mathfrak{D}}(m,n) + \zeta^{\mathfrak{m}}_{\mathfrak{D}}(n,m) = 0 \quad \text{for all } m,n \geq 2 \qquad (1.15)$$

In general, it reduces to the ordinary shuffle relation on the indices n_i of (1.4). The linearized double shuffle relations are therefore:

$$\begin{aligned} \zeta^{\mathfrak{m}}_{\mathfrak{D}}(w \sqcup\!\sqcup w') &= 0 \quad \text{for all } w, w' \in \{e_0, e_1\}^{\times} \\ \zeta^{\mathfrak{m}}_{\mathfrak{D}}(y \sqcup\!\sqcup y') &= 0 \quad \text{for all } y, y' \in \{1, 2, \ldots, \}^{\times} \\ \zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n) &= 0 \quad \text{for all } n \geq 1 \end{aligned} \qquad (1.16)$$

The first set of equations are the regularized shuffle relations as before, the second equations are obtained by shuffling the indices n_i in $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r)$. Racinet proved that the regularized double shuffle relations are motivic [17], and one can deduce that (1.16) are motivic. Therefore, the solutions to the relations (1.16) define a subspace $\mathfrak{ls} \subset \mathcal{U}\mathfrak{g}$ and an inclusion of bigraded Lie algebras for the Ihara bracket:

$$\mathfrak{dg}^{\mathfrak{m}} \subset \mathfrak{ls} \ .$$

A conjecture in [13], §8 amounts to the statement $\mathfrak{dg}^{\mathfrak{m}} \cong \mathfrak{ls}$. The main result of this paper is the construction of the missing exceptional generators in the algebra $\mathfrak{ls}$.

Theorem 1.4. *There is an explicit injective linear map*

$$\mathsf{e} : \mathsf{S}_{2n} \longrightarrow \mathfrak{ls}_4 \ . \qquad (1.17)$$

The formula for the map e is given in §8, and associates to every even period polynomial P an integral solution of the linearized double shuffle relations. The question of whether the elements e_P are motivic, i.e., whether they lie in $\mathfrak{dg}^{\mathfrak{m}}$, is open. Assuming this, we propose the following reformulation of (1.5):

Conjecture 2. (Broadhurst-Kreimer v2). The image of e lies in $\mathfrak{dg}^{\mathfrak{m}}$, and

$$
\begin{aligned}
H_1(\mathfrak{dg}^{\mathfrak{m}};\mathbb{Q}) &\cong \bigoplus_{i\geq 1}\overline{\sigma}_{2i+1}\mathbb{Q}\oplus\bigoplus_{n}\mathsf{e}(\mathsf{S}_{2n}) \\
H_2(\mathfrak{dg}^{\mathfrak{m}};\mathbb{Q}) &\cong \bigoplus_{n}\mathsf{S}_{2n} \\
H_i(\mathfrak{dg}^{\mathfrak{m}};\mathbb{Q}) &= 0 \quad \text{for} \quad i\geq 3\ .
\end{aligned}
\tag{1.18}
$$

In fact, by theorem 1.3, conjecture 2 holds if the e_P lie in $\mathfrak{dg}^{\mathfrak{m}}$, and if the Lie subalgebra of $\mathfrak{dg}^{\mathfrak{m}}$ generated by $\overline{\sigma}_{2i+1},\mathsf{e}_P$ has the homology (1.18). Since the elements $\overline{\sigma}_{2i+1}$, e_P and the Lie bracket are totally explicit, this part of the conjecture is elementary. For the first part, which claims that the elements e_P are motivic, it is enough to show that their class in $\mathfrak{ls}_4^{ab}$ lies in the image of (1.14). This is closely related to a question posed by Ihara (see the examples 8.4). In small weights, we find that the two maps $\mathsf{e}^{ab}, d:\mathsf{S}\rightarrow\mathfrak{ls}_4$ differ by an automorphism of S which involves numerators of Bernoulli coefficients, and should be related to arithmetic questions in Galois cohomology [16].

We show in §9.2 that conjecture 2 implies (1.5). If true, then (1.18) describes all relations between depth-graded motivic multiple zeta values (modulo $\zeta^{\mathfrak{m}}(2)$): a linear relation of weight N and depth d is true if and only if it holds amongst the coefficients of all Lie brackets of the elements $\overline{\sigma}_{2i+1}$ and e_P of the same weight and depth (see example 8.3).

1.5. **Contents of the paper.** In sections §§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 representations to replace words of fixed $\mathfrak{D}$-degree r in e_0, e_1 with polynomials in r variables:

$$\overline{\rho}: e_1e_0^{n_1}\ldots e_1e_0^{n_r} \quad\mapsto\quad x_1^{n_1}\ldots x_r^{n_r}\ .$$

This replaces identities between non-commutative formal power series with functional equations in commutative polynomials, reminiscent of the work of Ecalle. In particular, the depth r part of the motivic Drinfel'd associator yields generating series

$$\overline{\rho}\,(\mathrm{gr}^r_{\mathfrak{D}}\Phi^{\mathfrak{m}}) = \sum_{n_1,\ldots,n_r}\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1,\ldots,n_r)\,x_1^{n_1-1}\ldots x_r^{n_r-1}$$

similar to those considered in [13]. We show that in the polynomial representation, the Ihara bracket has an extremely simple form (§6.5). The generators (1.12) are simply

$$\overline{\rho}(\overline{\sigma}_{2n+1}) = x_1^{2n}\ .$$

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

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

which defines the exceptional elements in $\mathfrak{ls}_4$. These elements satisfy some remarkable properties, of which we only scratch the surface here. In §9 we discuss conjecture 2 and its consequences, and in §10 we discuss some applications for the enumeration of the totally odd multiple zeta values $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n_1+1,\ldots,2n_r+1)$.

We do not discuss conjecture 2 *per se* in this paper, and we make no mention of Goncharov's somewhat different conjectural description [9] of the depth filtration in terms of the cohomology of $GL_d(\mathbb{Z})$, since we have no understanding of its connection to (1.18). Ultimately, we believe that a full, geometric, understanding of conjecture 2 should come from studying the motivic fundamental groups of $\mathfrak{M}_{1,n}$ (via Grothendieck's two-tower principle) and in particular using multiple elliptic zeta values, which are the limits at tangential base points of the multiple elliptic polylogarithms defined in [4].

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:

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

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

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

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 $ш : \mathbb{Q}\langle e^0,e^1\rangle\otimes_{\mathbb{Q}}\mathbb{Q}\langle e^0,e^1\rangle\rightarrow \mathbb{Q}\langle e^0,e^1\rangle$. 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 ${}_0\Pi_1(\mathbb{Q})$ (corresponding to the group structure on ${}_0\Pi_1(\mathbb{Q})$, which exists because in the de Rham realisation there is a canonical path between any two points on X) is the completed Lie algebra $\mathfrak{g}^\wedge$ of the graded Lie algebra $\mathfrak{g}$ which is freely generated by the two elements e_0,e_1 in degree minus one. The universal enveloping algebra of $\mathfrak{g}$ is the tensor algebra on e_0,e_1:

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

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.

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 $\mathcal{G}_{MT}$ denote the group of automorphisms of the fiber functor, which is an affine group scheme over $\mathbb{Q}$. It has a decomposition as a semi-direct product

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

where $\mathcal{U}_{MT}$ 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 $\mathcal{U}_{MT}$ 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 $\mathcal{U}^{ab}_{MT}$ 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

$$\mathcal{U}_{MT} \times {}_0\Pi_1 \longrightarrow {}_0\Pi_1 \ . \tag{2.2}$$

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

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

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 Y. Ihara. It is obtained from [8], §5.9, §5.13 by reversing all words in order to be consistent with our conventions for iterated integrals. Given $a \in {}_0\Pi_1$, its action on an element $g \in {}_0\Pi_1$ is

$$a \circ g = \langle a \rangle_0(g)\, a \ , \tag{2.5}$$

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

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

Definition 2.1. Define a $\mathbb{Q}$-bilinear map

$$\underline{\circ} : \mathcal{U}\mathfrak{g} \otimes_{\mathbb{Q}} \mathcal{U}\mathfrak{g} \rightarrow \mathcal{U}\mathfrak{g}$$

inductively as follows. For any words a, w in e_0, e_1, and for 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 $a_i \in \{e_0, e_1\}^{\times}$, $(a_1 \ldots a_n)^* = (-1)^n a_n \ldots a_1$.

The map $\underline{\circ}$ is a linearisation of the full action $\circ : \mathcal{U}\mathfrak{g} \otimes_{\mathbb{Q}} \mathcal{U}\mathfrak{g} \rightarrow \mathcal{U}\mathfrak{g}$ induced by (2.2).

Proposition 2.2. *Let $\circ$ also denote the action*

$$\mathfrak{g} \otimes_{\mathbb{Q}} \mathcal{U}\mathfrak{g} \rightarrow \mathcal{U}\mathfrak{g} \tag{2.8}$$

induced by (2.2). *If $i : \mathfrak{g} \rightarrow \mathcal{U}\mathfrak{g}$ is the natural map, then $a \circ b = i(a) \,\underline{\circ}\, b$.*

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 $\mathfrak{g}$ with its image in $\mathcal{U}\mathfrak{g}$, it follows that the infinitesimal, weight-graded, version of the map (2.6) is the derivation $\langle f \rangle_0 : \mathfrak{g} \rightarrow \mathfrak{g}$ which for any $f \in \mathfrak{g}$ is given by

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

Thus $\langle f \rangle_0 : \mathcal{U}\mathfrak{g} \rightarrow \mathcal{U}\mathfrak{g}$ is the map

$$\langle f \rangle_0 \,(e_0^{m_0} e_1 \ldots e_1 e_0^{m_r}) = e_0^{m_0} f e_1 \ldots e_1 e_0^{m_r} + \ldots + e_0^{m_0} e_1 \ldots e_1 f^* e_0^{m_r} \ .$$

Concatentating on the right by f gives precisely the map defined by (2.7). □

2.3. **The motivic Lie algebra.** By equation (2.3), we obtain a map of Lie algebras

$$\mathrm{Lie}^{gr}(\mathcal{U}_{MT}) \longrightarrow \mathfrak{g} \ . \tag{2.9}$$

It follows from theorem 1.1 that this map is injective [1]. In this paper, we shall identify $\mathrm{Lie}^{gr}(\mathcal{U}_{MT})$ 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 $\mathcal{U}_{MT}$. Dualizing (2.2) gives the motivic coaction:

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

Furthermore, the de Rham image of the straight path dch from 0 to 1 in X defines the Drinfel'd associator element $\Phi \in {}_0\Pi_1(\mathbb{R})$ which begins

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

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 [1]: 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 $\omega_0 = \frac{dt}{t}$ and $\omega_1 = \frac{dt}{1-t}$.

Definition 3.1. The algebra of motivic multiple zeta values is defined as follows. The ideal of motivic relations between MZV's 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 $\mathcal{H}$.

Then $\mathcal{H}$ is naturally graded by the weight, 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.

3.1. **The Ihara coaction.** For any graded Hopf algebra H, let $IH = H_{>0}/H^2_{>0}$ denote the Lie coalgebra of indecomposable elements of H, and let $\pi : H_{>0} \to IH$ denote the natural map. Dualizing (2.8) 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 3.2. *For all $r \geq 1$, and $a_1,\dots,a_n \in \{0,1\}$, it is given by:*

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

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

Proof. It is almost immediate from (2.7) that this formula is dual to $\underline{\circ}$. □

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 $\mathcal{H}$ (resp. $\mathcal{A}$). 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 [1]).

4. The depth filtration

The inclusion $\mathbb{P}^1\backslash\{0,1,\infty\} \hookrightarrow \mathbb{P}^1\backslash\{0,\infty\}$ induces a map on the motivic fundamental groupoids ([8], §6.1)

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

and hence on the de Rham realisations

$$\mathcal{O}(\pi_1^{dR}(\mathbb{G}_m, \overrightarrow{1}_0, -\overrightarrow{1}_1)) \longrightarrow \mathcal{O}({}_0\Pi_1)$$

which is simply the inclusion of $\mathbb{Q}\langle e^0\rangle$ into $\mathbb{Q}\langle e^0, e^1\rangle$. The cokernel generates, via the deconcatenation coproduct, an increasing filtration called the depth:

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

with respect to which $\mathcal{O}({}_0\Pi_1)$ is a filtered Hopf algebra. Furthermore, since the map (4.1) is motivic, the depth filtration is preserved by the coaction (3.1) (which also follows by direct computation), and descends to the algebra $\mathcal{H}$.

Following [7], 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.

Definition 4.1. The depth filtration $\mathfrak{D}_d\mathcal{H}$ is the increasing filtration defined by

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

Likewise, 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 $\mathrm{gr}^{\mathfrak{D}}_r\mathcal{H}$.

The proof of proposition 5.8 in [7] gives a non-canonical isomorphism

$$\mathrm{gr}^{\mathfrak{D}}\mathcal{H} \cong \mathrm{gr}^{\mathfrak{D}}\big(\mathcal{A} \otimes_{\mathbb{Q}} \bigoplus_{n\geq 1} \zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n)\,\mathbb{Q}\big) \ , \tag{4.3}$$

where $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n) \in \mathrm{gr}^{\mathfrak{D}}_1\mathcal{H}$. We will show in proposition 6.4, following [13], that $\mathrm{gr}^{\mathfrak{D}}\mathcal{A}$ vanishes in bidegree (N,r) if N and r have different parity. In particular,

$$\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1,\ldots,n_r) \equiv 0 \pmod{\mathrm{gr}^{\mathfrak{D}}_{r-1}\mathcal{H} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)]} \tag{4.4}$$

if $n_1 + \ldots + n_r - r \equiv 1 \pmod 2$.

The depth filtration defines an increasing filtration on $\mathfrak{g}^{\mathfrak{m}}$ and $\mathcal{U}\mathfrak{g}^{\mathfrak{m}}$, which is induced by the grading on $T(\mathbb{Q}e_0 \oplus \mathbb{Q}e_1)$ for which e_0 has degree 0, and e_1 has degree -1. We denote the associated graded Lie algebra by $\mathfrak{dg}^{\mathfrak{m}}$.

Remark 4.2. From now on, we shall replace the depth on the Lie algebra $\mathfrak{dg}^{\mathfrak{m}}$ with its opposite, giving a decreasing filtration $\mathfrak{D}^r$ on $\mathfrak{g}^{\mathfrak{m}}$ consisting of words with at least r occurrences of e_1. This is more or less standard in the literature. Therefore:

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

and all depths will always be non-negative. By (4.4), it follows that the components of $\mathfrak{dg}^{\mathfrak{m}}$ for which the weight and depth have different parity are zero.

5. Linearized double shuffle relations

5.1. **Reminders on the standard relations.** We briefly review the double shuffle relations and their depth-linearized versions. One should emphasize that the particular form of these equations is not of any importance: in this paper they are only used as a means of finding candidate motivic elements amongst their solutions.

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 $ш$. It is defined recursively by

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

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 $1 ш w = w ш 1 = w$. 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 $\Phi_w \Phi_{w'} = \Phi_{w ш w'}$ for all $w, w' \in \{e_0, e_1\}^\times$, 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 $\Delta_ш$ with respect to which e_0 and e_1 are primitive (compare §2.1). In other words, there is an equivalence:

$$\Phi_w \Phi_{w'} = \Phi_{w ш w'} \text{ for all } w, w' \iff \Phi \in \mathbb{Q}\langle\langle e_0, e_1\rangle\rangle^\times \text{ and } \Delta_ш \Phi = \Phi \widehat{\otimes} \Phi \tag{5.2}$$

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

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

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 (see remark 4.2). The relations (5.1), (5.2), (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 $\Phi \in \mathrm{gr}^r_{\mathfrak{D}} \mathcal{U}\mathfrak{g}_N$. It defines a linear form $w \mapsto \Phi_w$ on words of weight N and $\mathfrak{D}$-degree r. It satisfies the *linearized shuffle relation* 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 [17]. 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 $w, w' \in Y^\times$, if and only if the series

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

is group-like for the (completed) coproduct $\Delta_* : \mathbb{Q}\langle\langle Y\rangle\rangle \to \mathbb{Q}\langle\langle Y\rangle\rangle \widehat{\otimes}_{\mathbb{Q}} \mathbb{Q}\langle\langle Y\rangle\rangle$ 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_*:

$$\Phi_w \Phi_{w'} = \Phi_{w * w'} \text{ for all } w, w' \quad \Longleftrightarrow \quad \Phi \in \mathbb{Q}\langle\langle Y\rangle\rangle^{\times} \text{ and } \Delta_* \Phi = \Phi \widehat{\otimes} \Phi \tag{5.6}$$

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

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

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

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 degree 1). By inspection of (5.4) it follows that

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

and the associated graded 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

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

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

Definition 5.2. Let $\Phi \in T(\mathbb{Q}Y)$ of degree N 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 relation* if

$$\Delta'_{ш} \Phi = 0$$

where $\Delta'_{ш}$ is the reduced coproduct of $\Delta_{ш}$ 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 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 [17], Racinet considered a certain graded vector space, denoted $\mathfrak{dm}_0(\mathbb{Q})$ (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 rôle here.

Definition 5.3. Let $\Phi \in \mathrm{gr}^{\mathfrak{D}}_r \mathcal{U}\mathfrak{g}_N$. The linear form $w \mapsto \Phi_w$ on words of weight N and $\mathfrak{D}$-degree r satisfies the *linearized double shuffle relations* if

$$\Delta_{ш} \Phi = 0 \qquad \text{and} \qquad \Delta_* \alpha(\Phi) = 0 \ .$$

When $r = 1$, we add the extra condition that $\Phi = 0$ when N is even. Let $\mathfrak{ls} \subset \mathcal{U}\mathfrak{g}$ denote the vector space of elements satisfying the linearized double shuffle relations.

Remark 5.4. There is a natural inclusion

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

As we shall see later, the vector spaces $\mathfrak{ls}_{n,d}$ are isomorphic to the vector spaces denoted $D_{n+d,d}$ in [13]. In [13] 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 [17] 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 proposition 2.2 in [17], but holds in $\mathfrak{ls}$ by definition 5.3). □

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 algebras:

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

where $\mathfrak{g}^{\mathfrak{m}}$ is the image of the (weight-graded) Lie algebra of $\mathcal{U}_{MT}$ and is isomorphic to the free graded Lie algebra on generators σ_{2i+1} for $i \geq 1$. A standard conjecture states that this 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. All the above Lie algebras can be viewed inside $\mathcal{U}\mathfrak{g} = T(\mathbb{Q}e_0 \oplus \mathbb{Q}e_1)$, which is graded for the $\mathfrak{D}$-degree.

Next we show that complicated expressions in the non-commutative algebra $\mathcal{U}\mathfrak{g}$ can be greatly simplified by encoding words of fixed $\mathfrak{D}$-degree in terms of polynomials.

6. Polynomial representations

6.1. **Composition of polynomials.** Recall from (2.1) that $\mathcal{U}\mathfrak{g}$ is isomorphic to the $\mathbb{Q}$-tensor algebra on e_0, e_1, and its subspace $\mathrm{gr}^r_{\mathfrak{D}} \, \mathcal{U}\mathfrak{g}$ of $\mathfrak{D}$-degree r is the subspace of elements with exactly r occurrences of e_1.

Definition 6.1. Consider the isomorphism of vector spaces

$$\begin{array}{rcl} \rho : \mathrm{gr}^r_{\mathfrak{D}} \, \mathcal{U}\mathfrak{g} & \longrightarrow & \mathbb{Q}[y_0, \ldots, y_r] \\ e_0^{a_0} e_1 e_0^{a_1} e_1 \ldots e_1 e_0^{a_r} & \mapsto & y_0^{a_0} \ldots y_r^{a_r} \end{array} \tag{6.1}$$

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

The operator $\underline{\circ} : \mathcal{U}\mathfrak{g} \otimes_{\mathbb{Q}} \mathcal{U}\mathfrak{g} \to \mathcal{U}\mathfrak{g}$ respects the $\mathfrak{D}$-grading, so clearly defines a map

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

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

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

Antisymmetrizing, we obtain a formula for the Ihara bracket

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

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

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 algebra $\mathfrak{g}^{\mathfrak{m}}\subset\mathfrak{g}\subset\mathcal{U}\mathfrak{g}$ is contained in the subspace of elements which are primitive with respect to the shuffle coproduct $\Delta_{Ш}$. Let $\pi_0:\mathcal{U}\mathfrak{g}\to\mathbb{Q}$ 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 $\partial_0:\mathcal{U}\mathfrak{g}\longrightarrow\mathcal{U}\mathfrak{g}$ which satisfies

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

for all non-negative integers $a_0,\ldots,a_r$. Let $r\geq1$, $\xi\in\mathrm{gr}^r_{\mathfrak{D}}\mathcal{U}\mathfrak{g}$, and $f=\rho(\xi)$. If ξ is primitive for $\Delta_{Ш}$, it satisfies $\partial_0\xi=0$ and the previous equation is

$$\sum_{i=0}^{r}\frac{\partial f}{\partial y_i}=0 \qquad (6.5)$$

This is equivalent to $dg=0$, where $g(y_0,\ldots,y_r)=f(y_0,\ldots,y_r)-f(y_0+\lambda,\ldots,y_r+\lambda)$, and hence f is translation invariant. □

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

$$
\begin{aligned}
\mathbb{Q}[y_0,\ldots,y_r] &\longrightarrow \mathbb{Q}[x_1,\ldots,x_r] \\
f &\mapsto \overline{f}
\end{aligned} \qquad (6.6)
$$

where $\overline{f}$ is the reduced polynomial $\overline{f}(x_1,\ldots,x_r)=f(0,x_1,\ldots,x_r)$. In the case when f is translation invariant, we have the equation

$$f(y_0,\ldots,y_r)=\overline{f}(y_1-y_0,\ldots,y_r-y_0) \qquad (6.7)$$

Taking the coefficients of (6.7) gives equation **I2** of [1], 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 $\overline{\rho}(\xi)\in\mathbb{Q}[x_1,\ldots,x_r]$.

To avoid confusion, we reserve the variables $x_1,\ldots,x_r$ for the reduced polynomial $\overline{\rho}(\xi)$ and use the variables $y_0,\ldots,y_r$ 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 $* : \mathcal{U}\mathfrak{g} \to \mathcal{U}\mathfrak{g}$ considered earlier. Restricting to $\mathfrak{D}$-degree r and transporting via ρ we obtain a map

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

Therefore, if $f \in \mathbb{Q}[y_0,\ldots,y_r]$ 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 $\mathsf{y}_{i_1}\ldots\mathsf{y}_{i_r} \mapsto (-1)^r \mathsf{y}_{i_r}\ldots\mathsf{y}_{i_1}$. This defines an involution

$$\begin{array}{rcl} \overline{\tau} : \mathbb{Q}[x_1,\ldots,x_r] & \longrightarrow & \mathbb{Q}[x_1,\ldots,x_r] \\ \overline{\tau}(\overline{f})(x_1,\ldots,x_r) & = & (-1)^r \overline{f}(x_r,\ldots,x_1) \end{array} \tag{6.10}$$

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

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

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 rôle in what follows.

6.4. **Parity relations.** The following result is well-known, and was first proved by Tsumura, and subsequently in ([14], theorem 7). We repeat the proof for convenience.

Proposition 6.4. *The components of* $\mathfrak{ls}$ *in weight* N *and depth* r *vanish unless* $N \equiv r$ mod 2. *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 [14], consider the relation

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

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. 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 line 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

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

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

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

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:

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

and anti-invariant under the reflections σ and τ. Thus $\mathbb{Q}f \subset \mathfrak{p}_r$ is isomorphic to the sign (orientation) representation 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 satisfing* (6.13). *Then the Ihara bracket is given by averaging over the dihedral symmetry group:*

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

In particular, $\{.,.\} : \mathfrak{p}_r \times \mathfrak{p}_s \rightarrow \mathfrak{p}_{r+s}$, 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 $r+s+1$. The Jacobi identity for $\{.,.\}$ is straightforward after identifying its terms with the set of double cuts in a polygon. □

A similar dihedral symmetry was also found by Goncharov [9]; 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. Alternatively, one can check that (6.5) is preserved by the bracket:

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

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

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

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

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

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

is an injective map of bigraded Lie algebras.

Definition 6.7. We use the notation $D_r \subset \mathbb{Q}[x_1,\ldots,x_r]$ to denote the space $\overline{\rho}(\mathfrak{ls}_r)$ in depth r. It is the space of polynomial solutions to the linearized double shuffle equations in depth r and was denoted $D_{\bullet,r}$ in [13].

6.6. **Generators in depth 1 and examples.** It follows from theorem 1.3 that in depth 1, the Lie algebra $\mathfrak{dg}^{\mathfrak{m}}$ has exactly one generator in every odd weight ≥ 3:

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

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

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

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

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

7. Modular relations in depth two

7.1. **Reminders on period polynomials.** We recall some definitions from ([15], §1.1). Let $S_{2k}(PSL_2(\mathbb{Z}))$ denote the space of cusp forms of weight $2k$ for the full modular group $PSL_2(\mathbb{Z})$.

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

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

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

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 theorem gives a map which associates, in particular, an even period polynomial to every cusp form:

$$S_{2k}(PSL_2(\mathbb{Z})) \longrightarrow W^e_{2k} \otimes_{\mathbb{Q}} \mathbb{C} \ .$$

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

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

where $+$ denotes the invariants under the involution $(X,Y) \mapsto (-X,Y)$. 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 codimension 1. Thus $\dim S_{2k}(PSL_2(\mathbb{Z})) = \dim \mathsf{S}_{2k}$ and it follows from classical results on the space of modular forms that:

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

7.2. **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 $\overline{\rho}$ leads to a map

$$D_1 \wedge D_1 \longrightarrow D_2 \ , \tag{7.6}$$

given by the formula in example 6.9. Since D_1 is isomorphic to the graded vector space $\mathbb{Q}[x_1^{2n}, n \geq 1]$, it follows that $D_1 \wedge D_1$ 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 (c.f., [9, 14, 19]) that

$$\ker(\{.,.\} : D_1 \wedge D_1 \longrightarrow D_2) \overset{\sim}{\longrightarrow} \mathsf{S} \ . \tag{7.7}$$

In fact, the dimensions of the space D_2 have been computed many times in the literature (for example, by some simple representation-theoretic arguments), and it is relatively easy to show [14] that the following sequence is exact:

$$0 \longrightarrow \mathsf{S} \longrightarrow D_1 \wedge D_1 \longrightarrow D_2 \longrightarrow 0 \ . \tag{7.8}$$

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 Ihara's relation

$$3\{x_1^4, x_2^6\} = \{x_1^2, x_2^8\} \ . \tag{7.9}$$

7.3. **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 Lie algebra $\mathrm{Lie}(V)$. The triple Ihara bracket gives a map

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

and hence a map $\mathrm{Lie}_3(D_1) \to D_3$ 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 D_3, and computed its dimensions in each weight. It follows from his work that the following sequence

$$0 \longrightarrow \mathsf{S} \otimes_{\mathbb{Q}} D_1 \longrightarrow \mathrm{Lie}_3(D_1) \longrightarrow D_3 \longrightarrow 0 \tag{7.10}$$

is exact, where the first map (identifying S with $\ker(\Lambda^2 D_1 \to D_2)$) is given by

$$\mathsf{S} \otimes_{\mathbb{Q}} D_1 \hookrightarrow \Lambda^2 D_1 \otimes_{\mathbb{Q}} D_1 \to \mathrm{Lie}_3(D_1) \ ,$$

where the second map is $[a, b] \otimes c \mapsto [a, b] \otimes c + a \otimes [c, b]$. Starting from depth 4, the structure of $\mathfrak{ls}_d \cong D_d$ is not known. In particular, it is easy to show that the map given by the quadruple Ihara bracket

$$\mathrm{Lie}_4(D_1) \longrightarrow D_4$$

is not surjective, since in weight 12, $\dim D_4 = 1$, but $\mathrm{Lie}_4(D_1) = 0$. 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 equality $\dim \mathsf{S} \otimes_{\mathbb{Q}} D_1 = \dim \Lambda^3(D_1)$ which follows from (7.4), and is presumably well-known.

8. Exceptional modular elements in depth four

8.1. **Linearized equations in depth four.** For the convenience of the reader, we write out the linearized double shuffle relations in full in depth four. For any set of indices $\{i,j,k,l\} = \{1,2,3,4\}$, and $f \in \mathbb{Q}[x_1,\ldots,x_4]$, we write:

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

Then D_4 (see [13], §8) is the subspace of polynomials $f \in \mathbb{Q}[x_1,\ldots,x_4]$ satisfying

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

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

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

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

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

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

8.2. **Definition of the exceptional elements.** Let $f \in \mathbb{Q}[x,y]$ 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

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

where $f_0 \in \mathbb{Q}[x,y]$ is symmetric of homogeneous 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 $f_1 = (x-y)f_0$. 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

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

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 $\overline{\mathsf{e}}_f \in \mathbb{Q}[x_1,\ldots,x_4]$ is obtained by setting $y_0 = 0, y_i = x_i$, for $i = 1,\ldots,4$.

Note that since f is even it vanishes to order two along $x, y, (x-y)$, and therefore f_0 also vanishes along $x=0, y=0$. One checks from definition (8.5) that

$$\overline{\mathsf{e}}_f(x,y,0,0) = f_1(x,y)\ , \tag{8.6}$$

which follows from a trivial calculation, and is related to the discussion in [5], §9.2.

Theorem 8.2. *The reduced polynomial $\overline{\mathsf{e}}_f$ obtained from (8.5) satisfies the linearized double shuffle relations. In particular, we get an injective linear map*

$$\overline{\mathsf{e}} : \mathsf{S} \longrightarrow D_4$$

Proof. The injectivity follows immediately from (8.6). The proof that the linearized double shuffle relations hold is a trivial but tedious calculation, and is left to the reader. Some pointers: the linearized stuffle relations (8.2) hold for the terms in f_1 and f_0 separately. For the terms in f_1 this uses the antisymmetry and parity properties with respect to x and y only, for the terms in f_0 this uses the 3-term relation (8.4). For the linearized shuffle relation, it is enough to show that if $g(x,y)$ is any symmetric polynomial satisfying $g(-x,y) = g(x,-y) = -g(x,y)$, then setting

$f_0(x,y) = (x+y)g(x,y)$, and $f_1(x,y) = (x^2-y^2)g(x,y)$ in (8.5) yields a solution to (8.3). It is clear that polynomials in S can be written in this form. $\square$

Identifying $\mathfrak{ls}_4$ with D_4 via the map $\overline{\rho}$, we can view e as a map from S to $\mathfrak{ls}_4$. Note that the 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 interesting to see if the five-fold symmetry of the elements e_f is related to the pentagon equation.

Example 8.3. 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. They are all motivic (see the examples in 8.4 below). We know by theorem 1.3 that $\mathfrak{g}^{\mathfrak{m}}$ is of dimension 2 in weight twelve, spanned by $\{\sigma_3, \sigma_9\}$ and $\{\sigma_5, \sigma_7\}$. We know by (7.9) that in weight twelve $\mathfrak{dg}_2^{\mathfrak{m}}$ is of dimension one, $\mathfrak{dg}_3^{\mathfrak{m}}$ vanishes by parity, so it follows that $\mathfrak{dg}_4^{\mathfrak{m}}$ is of dimension one and hence spanned by $\overline{\mathsf{e}}_{12}$. Writing out just a few of its coefficients as an example, we have:

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

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

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

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

8.3. **Are the exceptional elements motivic?** One way to show that the exceptional elements e_f are motivic would be to show that their classes in $\mathfrak{ls}_4$ modulo commutators are in the image of the following map:

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

where $\mathsf{S} \subset \Lambda^2 \mathfrak{dg}_1^{\mathfrak{m}}$ 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.

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

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

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

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

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

$$d\xi = \{\sigma_i^{(1)}, \sigma_j^{(3)}\} + \{\sigma_i^{(2)}, \sigma_j^{(2)}\} + \{\sigma_i^{(3)}, \sigma_j^{(1)}\}\ ,$$

where $\{.,.\} : \bigwedge^2 \mathfrak{g}^{\mathfrak{m}} \to \mathfrak{g}^{\mathfrak{m}}$ is the (full, i.e., not depth-graded) Ihara bracket.

Examples 8.4. The elements $\widetilde{\sigma}_3, \widetilde{\sigma}_5, \widetilde{\sigma}_7, \widetilde{\sigma}_9$ 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

$$\{\widetilde{\sigma}_3, \widetilde{\sigma}_9\} - 3\{\widetilde{\sigma}_5, \widetilde{\sigma}_7\} = \frac{691}{144}\, \mathsf{e}_{12} \mod \text{depth } \geq 5 \ , \tag{8.7}$$

which proves that the element e_{12} is motivic. An inspection of the proof of proposition 6.4 shows that the corresponding congruence

$$\{\widetilde{\sigma}_3, \widetilde{\sigma}_9\} - 3\{\widetilde{\sigma}_5, \widetilde{\sigma}_7\} \equiv 0 \mod 691 \ ,$$

propagates to depth five also. Compare with the 'key example' of [10], page 258, and the ensuing discussion. Thereafter, one checks that

$$\begin{aligned} d\big(2\,\sigma_3 \wedge \sigma_{13} - 7\,\sigma_5 \wedge \sigma_{11} + 11\,\sigma_7 \wedge \sigma_9\big) &\equiv \frac{3617}{720}\mathsf{e}_{16} \mod \{\mathfrak{g}_1^{\mathfrak{m}}, \mathfrak{g}_3^{\mathfrak{m}}\} \\ d\big(8\,\sigma_3 \wedge \sigma_{15} - 25\,\sigma_5 \wedge \sigma_{13} + 26\,\sigma_7 \wedge \sigma_{11}\big) &\equiv \frac{43867}{9000}\mathsf{e}_{18} \mod \{\mathfrak{g}_1^{\mathfrak{m}}, \mathfrak{g}_3^{\mathfrak{m}}\} \\ d\big(3\,\sigma_3 \wedge \sigma_{17} - 10\,\sigma_5 \wedge \sigma_{13} + 14\,\sigma_7 \wedge \sigma_{13} - 13\,f_9 \wedge f_{11}\big) &\equiv \frac{174611}{35280}\mathsf{e}_{20} \mod \{\mathfrak{g}_1^{\mathfrak{m}}, \mathfrak{g}_3^{\mathfrak{m}}\} \end{aligned}$$

and 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 $\zeta(20)\pi^{-20}$. Note that it does not seem possible to construct canonical associators $\widetilde{\sigma}_{2n+1}$ for $n \geq 5$ in a consistent way such that the above relations hold exactly in $\mathfrak{g}_4^{\mathfrak{m}}$.

Constructing elements $\sigma_{2i+1}^{(3)}$ is problematic since they are non-canonical, and have increasingly large prime factors in the denominators. Nonetheless, I can construct them all semi-explicitly, so the seemingly mysterious question of whether the elements e_f are motivic can be reduced to a concrete but complicated computation.

If the elements e_f can be shown to be motivic, then they provide in particular an answer to the question raised by Ihara in ([10], end of §4 page 259). The appearance of the numerators of Bernoulli numbers is related to conjecture 2 in [10] and has been studied from the Galois-theoretic side by Sharifi [18] and McCallum and Sharifi [16].

8.4. **Some properties of e_f.** The exceptional elements e_f satisfy many remarkable properties, and I will only outline a few of them here. The proofs are trivial yet sometimes lengthy applications of the definitions, basic properties of period polynomials, and the definition of $\{.,.\}$. For any polynomial $f \in \mathbb{Q}[x_1, \ldots, x_r]$, let

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

and denote the projection onto the even part in x_i by:

$$\pi_i^+ f = \sum_{k \geq 0} \pi_i^{2k} f \ .$$

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

$$\pi_0^+ \pi_1^+ \pi_2^+ \pi_3^+ \pi_4^+ (\mathsf{e}_f) = 0 \ . \tag{8.8}$$

We shall see later in §10.1 that this property is motivic, i.e., is stable under the Ihara bracket, and is related to the totally odd zeta values.

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

$$\frac{\partial^5}{\partial y_0 \partial y_1 \partial y_2 \partial y_3 \partial y_4}(\mathsf{e}_f) = 0 \ . \tag{8.9}$$

In other words, every monomial occurring in e_f only depends on four out of five of the variables $y_0, \ldots, y_4$. One can show that this property is also motivic: i.e., the set of polynomials in $f \in \mathfrak{p}_r$ annihilated by $\frac{\partial^{r+1}}{\partial y_0 \ldots \partial y_r}$ forms an ideal for the bracket $\{.,.\}$. In fact, there are many 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 $\overline{\mathfrak{p}}$ spanned by the x_1^{2n} and the $\overline{\mathsf{e}}_f$.

(3) The above two properties say that almost all the coefficients of e_f are zero. If we define the interior of a polynomial $p \in \mathbb{Q}[x_1, \ldots, x_r]$ to be $p^o = \pi_1^{\geq 2} \ldots \pi_r^{\geq 2} p$, then the majority of the non-trivial monomials in $\overline{\mathsf{e}}_f$ are determined by:

$$(\overline{\mathsf{e}}_f)^o = f_1(x_4 - x_3, x_2 - x_1)^o \ . \tag{8.10}$$

(4) Suppose that $f^{(1)}, \ldots, f^{(n)}$ are period polynomials, and let $f_1^{(i)}$ be as defined in §8.2. Then, generalizing (8.6), we have

$$\pi^0_{n+2} \ldots \pi^0_{4n} \big(\overline{\mathsf{e}}_{f^{(1)}} \circ (\overline{\mathsf{e}}_{f^{(2)}} \circ \ldots (\overline{\mathsf{e}}_{f^{(n-1)}} \circ \overline{\mathsf{e}}_{f^{(n)}}) \cdots)\big) = \prod_{i=1}^{n} f_1^{(i)}(x_i, x_{i+1}) \tag{8.11}$$

Unfortunately, some information about the polynomials f_i is lost in (4), but one can do better by using the operators π^+. For example, one checks that:

$$\pi_1^+ \pi_5^+ \pi_6^0 \pi_7^0 \pi_8^0 \left(\overline{\mathsf{e}}_f \circ \overline{\mathsf{e}}_g\right) = \big(\pi_1^+ \pi_4^0 \overline{\mathsf{e}}_f(x_1, x_2, x_3, x_4)\big) \times \big(\pi_5^+ \pi_6^0 \overline{\mathsf{e}}_g(x_3, x_4, x_5, x_6)\big) \tag{8.12}$$

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

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

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

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

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 that there are no non-trivial relations between the commutators $\{\overline{\mathsf{e}}_f, \overline{\mathsf{e}}_g\}$. Since similar factorization properties as (8.12) hold in higher orders, one might hope to prove, in a similar manner, that the Lie algebra generated by the exceptional elements e_f is free.

9. Lie algebra structure and Broadhurst-Kreimer conjecture

9.1. **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 (1.5), and Zagier's conjecture which states that the double shuffle relations generate all relations between multiple zeta values, it is natural to rephrase their conjectures in the Lie algebra setting as follows:

Conjecture 3. (Strong Broadhurst-Kreimer and Zagier conjecture)

$$\begin{aligned} H_1(\mathfrak{ls}, \mathbb{Q}) &\cong \mathfrak{ls}_1 \oplus \mathsf{e}(\mathsf{S}) \\ H_2(\mathfrak{ls}, \mathbb{Q}) &\cong \mathsf{S} \\ H_i(\mathfrak{ls}, \mathbb{Q}) &= 0 \quad \text{for all} \quad i \geq 3 \ . \end{aligned} \tag{9.1}$$

This conjecture is the strongest possible conjecture that one could make: as we shall see below, it implies nearly all the remaining open problems in the field. The numerical evidence for this conjecture is substantial [5], 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 4. (Motivic version of the Broadhurst-Kreimer conjecture). The exceptional elements e_f are motivic (i.e., $\mathsf{e}_f \in \mathfrak{dg}^{\mathfrak{m}}$), and

$$\begin{array}{rcl} H_1(\mathfrak{dg}^{\mathfrak{m}}, \mathbb{Q}) & \cong & \mathfrak{dg}^{\mathfrak{m}}_1 \oplus \mathsf{e}(\mathsf{S}) \\ H_2(\mathfrak{dg}^{\mathfrak{m}}, \mathbb{Q}) & \cong & \mathsf{S} \\ H_i(\mathfrak{dg}^{\mathfrak{m}}, \mathbb{Q}) & = & 0 \quad \text{for all} \quad i \geq 3 \ . \end{array} \tag{9.2}$$

Since the conjectural generators are totally explicit, it is possible to verify the independence of Lie brackets in the reduced polynomial representation $\overline{\rho}(\mathfrak{g}^{\mathfrak{m}})$ simply by computing the coefficients of a small number of monomials. In this way, it should be possible to verify (9.2) 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.

9.2. **Enumeration of dimensions.** Let $\mathfrak{g}$ be a Lie algebra over a field k, and let $\mathcal{U}\mathfrak{g}$ be its universal enveloping algebra. Let $\varepsilon : \mathcal{U}\mathfrak{g} \rightarrow k$ denote the augmentation map. Recall that the Chevalley-Eilenberg complex ([20], §7.7):

$$\cdots \longrightarrow \mathcal{U}\mathfrak{g} \otimes_k \Lambda^2 \mathfrak{g} \longrightarrow \mathcal{U}\mathfrak{g} \otimes_k \mathfrak{g} \longrightarrow \mathcal{U}\mathfrak{g} \overset{\varepsilon}{\longrightarrow} k \longrightarrow 0 \tag{9.3}$$

is exact in all degrees, and hence defines a resolution of k. Viewing k as a $\mathcal{U}\mathfrak{g}$-module via ε, and applying the functor $M \mapsto k \otimes_{\mathcal{U}\mathfrak{g}} M$ to (9.3) gives the standard complex

$$\cdots \longrightarrow \Lambda^3 \mathfrak{g} \longrightarrow \Lambda^2 \mathfrak{g} \longrightarrow \mathfrak{g} \longrightarrow k \longrightarrow 0 \tag{9.4}$$

whose homology groups in degree i are, by definition, $H_i(\mathfrak{g}, k)$.

Now suppose that $\mathfrak{g}$ is bigraded, and finite-dimensional in each bigraded piece. Then $\Lambda^i \mathfrak{g}, \mathcal{U}\mathfrak{g}$ inherit a bigrading too. For any bigraded $\mathfrak{g}$-module M, 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 modules M^l, $l \geq 0$, we set

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

Writing $\Lambda^1 \mathfrak{g} = \mathfrak{g}$, and $\Lambda^0 \mathfrak{g} = k$, the exactness of (9.3) yields

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

But by (9.4), $\mathcal{X}_{\Lambda^\bullet \mathfrak{g}}(-1,s,t) = \mathcal{X}_{H_\bullet(\mathfrak{g})}(-1,s,t)$ and we conclude that

$$\mathcal{X}_{\mathcal{U}\mathfrak{g}}(s,t) = \frac{1}{\mathcal{X}_{H_\bullet(\mathfrak{g})}(-1,s,t)} \ . \tag{9.5}$$

9.3. **Corollaries of conjectures 3 and 4.** Let us first apply §9.2 to the algebra $\mathfrak{ls}$, bigraded by weight and depth. Assuming conjecture 3, and from (7.4), we would have

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

where $\mathbb{O}$ and $\mathbb{S}$ were defined in (1.6), and (9.5) implies that

$$\mathcal{X}_{\mathcal{U}\mathfrak{ls}}(s,t) = \frac{1}{1-\mathbb{O}(s)\,t + \mathbb{S}(s)\,t^2 - \mathbb{S}(s)\,t^4}\ , \tag{9.6}$$

Identifying $\mathfrak{ls}_d$ via the isomorphism $\overline{\rho}$ with the space of polynomials D_d satisfying the linearized double shuffle relations, we obtain the formula stated in ([13], appendix).

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

$$\dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{g}^{\mathfrak{m}})_{N,d} \leq \dim_{\mathbb{Q}}(\mathcal{U}\mathfrak{ls})_{N,d}\ . \tag{9.7}$$

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 1.3 that

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

Likewise, specializing (9.6) to $t=1$ we obtain

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

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 (9.7) are non-negative, this implies equality in (9.7). We have shown that conjecture 1 implies that $\mathfrak{dg}^{\mathfrak{m}} = \mathfrak{ls}$, and so evidently:

Proposition 9.1. *Conjecture 3 is equivalent to:*

$$\textit{Conjecture } 4 \quad \textit{plus} \quad \mathfrak{dg}^{\mathfrak{m}} = \mathfrak{ls}\ .$$

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 (equivalent to a conjecture of Zagier's). By Furusho's theorem [12], it would in turn imply Drinfeld's conjecture that all relations between (motivic) multiple zeta values are generated by the associator relations.

Corollary 9.2. *Conjecture 4 implies a Broadhurst-Kreimer conjecture for motivic multiple zeta values. More precisely, conjecture 4 implies that*

$$\sum_{N,d\geq 0}(\dim_{\mathbb{Q}}\mathrm{gr}^{\mathfrak{D}}_d\mathcal{H}_N)\,s^N t^d = \frac{1+\mathbb{E}(s)t}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2-\mathbb{S}(s)t^4}\ . \tag{9.8}$$

Proof. Apply §9.2 to $\mathfrak{dg}^{\mathfrak{m}}$. Then conjecture 4 implies via (9.5) that

$$\sum_{N,d\geq 0}(\dim_{\mathbb{Q}}\mathrm{gr}^d_{\mathfrak{D}}\mathcal{U}\mathfrak{g}^{\mathfrak{m}}_N)s^N t^d = \frac{1}{1-\mathbb{O}(s)\,t+\mathbb{S}(s)\,t^2-\mathbb{S}(s)\,t^4}\ . \tag{9.9}$$

Equation (9.8) follows from (4.3), which gives

$$\mathrm{gr}^{\mathfrak{D}}_d\mathcal{H} \cong \mathrm{gr}^{\mathfrak{D}}_d\big(\mathcal{A}\otimes_{\mathbb{Q}}\mathbb{Q}[\zeta^{\mathfrak{m}}(2)]\big) \cong \mathrm{gr}^{\mathfrak{D}}_d\mathcal{A} \oplus \big(\mathrm{gr}^{\mathfrak{D}}_{d-1}\mathcal{A}\otimes_{\mathbb{Q}}\bigoplus_{n\geq 1}\zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n)\mathbb{Q}\big)\ .$$

The statement follows from the fact that $\mathrm{gr}^{\mathfrak{D}}\mathcal{A} \cong (\mathrm{gr}_{\mathfrak{D}}\mathcal{U}\mathfrak{g}^{\mathfrak{m}})^{\vee}$. □

Remark 9.3. Conjecture 4 is in turn equivalent to the statement that the e_P are motivic, and that the Lie subalgebra of $\mathfrak{dg}^{\mathfrak{m}}$ generated by the elements x_1^{2n} and e_P has the homology given by (9.2).

10. Totally odd multiple zeta values

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

$$\zeta^{\mathfrak{m}}(2n_1+1,\ldots,2n_r+1) \ , \tag{10.1}$$

where $n_1,\ldots,n_r$ are integers ≥ 1. Then $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{odd} \subset \mathrm{gr}^{\mathfrak{D}}\mathcal{H}$ is the vector subspace spanned by the depth-graded versions of (10.1). It is clear from the linearized stuffle product formula that $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{odd}$ is an algebra, indeed, it is a quotient of the shuffle algebra

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

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

Proposition 10.1. *The space $\mathcal{H}^{odd}$ is almost stable under the motivic coaction:*

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

Furthermore, the group U^{dR} acts trivially on the associated graded $\mathrm{gr}^{\mathfrak{D}}\mathcal{H}^{odd}$.

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

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

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:

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

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

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

In this case, the quotient sequence has the property that every pair of consecutive 1's are separated by an even number of 0's, which defines an element of $\mathcal{H}^{odd}$. 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. □

It follows immediately from the proposition that the action of the graded Lie algebra $\mathrm{Lie}^{gr}U^{dR}$ on the two-step quotients $\mathfrak{D}_r\mathcal{H}^{odd}/\mathfrak{D}_{r-2}\mathcal{H}^{odd}$ factors through its abelianization $\mathrm{Lie}^{gr}(U^{dR})^{ab}$, which has canonical generators in every odd degree $2r+1$, for $r\geq 1$. Thus for every integer $n\geq 1$, there is a well-defined derivation

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

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

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

where, by duality,

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

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

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

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 $\mathfrak{g}$.

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 $|S_{N,r}|$ square matrix whose entries are the integers

$$(C_{N,r})_{i,j} = c_{\binom{s_i}{s_j}} \ , \quad s_i, s_j \in S_{N,r} \ . \tag{10.2}$$

10.1. **Enumeration of totally odd multiple zeta values.**

Definition 10.2. We say that a polynomial $f \in \mathbb{Q}[y_0, y_1, \dots, y_r]$ is *uneven* if the coefficient of $y_0^{2n_0} \dots y_r^{2n_r}$ in f vanishes for all $n_0, \dots, n_r \geq 0$.

Recall from (8.8) that the exceptional elements $e_f \in \mathfrak{ls}$ are uneven. The following proposition is a sort of dual to the previous one.

Proposition 10.3. *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 $y_0^{2n_0} \dots y_N^{2n_N}$ in $\{f, g\}$ is a linear combination of the coefficients of totally even monomials in f, which all vanish. □

It follows from the above that the Lie ideal in $\mathfrak{ls}$ generated by the exceptional elements is orthogonal to $\mathrm{gr}^{\mathfrak{D}} \mathcal{A}^{odd}$. In the light of conjecture 4 it is therefore natural to expect that $\mathrm{gr}^{\mathfrak{D}} \mathcal{A}^{odd}$ is dual to $\mathfrak{g}^{odd}$, which suggests the following:

Conjecture 5. ('Uneven' part of motivic Broadhurst-Kreimer conjecture)

$$\sum_{N \geq 0, d \geq 0} (\dim_{\mathbb{Q}} \mathrm{gr}_d^{\mathfrak{D}} \mathcal{A}_N^{od}) s^N t^d = \frac{1}{1 - \mathbb{O}(s) t + \mathbb{S}(s) t^2} \ . \tag{10.3}$$

Since the action of the operators ∂_{2n+1} on the totally odd zeta values can be computed explicitly in terms of binomial coefficients, one can hope to prove this conjecture by elementary methods. Indeed, the left-hand side of (10.3) 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 (10.2). Using this formulation, I have verified (10.3) up to weight 30. It would be desirable to have an interpretation of (10.3) in terms of multiple elliptic zeta values [4], which place modular forms and multiple zeta values on an equal footing.

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

$$\sum_{N\geq 0, d\geq 0} \dim_{\mathbb{Q}} \mathcal{Z}^{odd}_{N,d} s^N t^d = \frac{1}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2} \ . \tag{10.4}$$

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