

# Rational structures of multiple zeta values

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## Introduction

This thesis aims to discuss and expand upon a collection of interrelated problems in number theory, all tying to the theory of multiple zeta values and Drinfel'd associators. Multiple zeta values provide a generalisation of the Riemann zeta function to multiple variables. Where questions of algebraic independence of values of the Riemann zeta function at integer values seem intractable, multiple zeta values have a rich algebraic structure. One interesting question in modern number theory is to describe explicitly this structure, giving all relations among multiple zeta values and describing the Hilbert Poincaré series of their graded  $\mathbb{Q}$ -span.

There are several equations describing relations among multiple zeta values, conjecturally describing all relations. The most interesting of these are Drinfel'd's *associator* equations: functional equations among power series in two non-commuting variables, with solution given by the generating series for multiple zeta values [15]. This adds an extra layer of interest to the study of multiple zeta values: it is known that there is a solution to the associator equations with rational coefficients. Knowing such an object explicitly would be an extremely powerful computational tool: it has applications in the theory of knot invariants [2], the construction of quasitriangular quasi-Hopf algebras, along with providing a tool for decomposition of multiple zeta values into a given basis [6]. This is where this thesis begins: can we find a rational associator, using multiple zeta values as a model for the coefficients? While we do not answer this question, it provides a start point for fruitful research.

Solving the associator equations directly proves quite challenging, so we turn to the second set of equations describing relations among multiple zeta values: the double shuffle equations. Arising naturally from the definition of multiple zeta values, these equations are much simpler, and are implied by the associator equations [19]. Conjecturally, they describe all relations among multiple zeta values, and are thus equivalent to the associator equations. Furthermore, they can easily be considered modulo products, or certain filtrations, allowing us to find relations among “graded” multiple zeta values, which can hopefully be lifted to true relations, reducing the problem of finding rational solutions to the double shuffle equations to that of finding rational solutions modulo products, or a filtration. Indeed, one can reduce many problems about the dimension of the vector space spanned by multiple zeta values to problems about these simplified spaces [7].

In solving these problems, we gain an additional geometric structure: multiple zeta values and the associator equations can be found in the geometry of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . By exploiting this geometric origin, we can produce a motivic Galois group with an action on (motivic) multiple zeta values, preserving relations. Thus, this Galois group has an action on (motivic) solutions to the associator and double shuffle equations, which we can exploit in order to attempt to find rational solutions, or to bound the dimension of certain spaces.

This is an incredibly rich and multifaceted problem, and as such, we must summarise it as best we can. The structure of this thesis will be as follows: In section one, we will condense the necessary background material. We first introduce multiple zeta values and their combinatorics, as these play a vital role in describing the object of interest: Drinfel'd associators. These formal power series satisfy certain equations and are used in the construction of quasitriangular quasi-Hopf algebras. However, they are quite mysterious: only a few examples are known explicitly, and all arise from other areas of mathematics, such as conformal field theory and knot theory. Thus, instead of studying associators directly, we study the Lie group  $\mathrm{DMR}_0$  of solutions to the double shuffle equations, allowing us to use the machinery of the motivic Galois group and its ties to  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ .

In section two, we consider the Lie algebra  $\mathfrak{dmt}_0$  associated to  $\mathrm{DMR}_0$ , and the equations describing it: the double shuffle equations modulo products. This Lie algebra contains a Lie algebra called the *motivic* Lie algebra, which contains Lie algebraic analogues of associators. It is a free Lie algebra with generators in every odd degree greater than 1, which act on the space

of associators, allowing us to produce infinitely many rational associators given one. However, these generators do not have canonical representations, so we discuss methods used to make them canonical: a Gram-Schmidt procedure using inner products, an approach using “polar” solutions, etc. We also briefly consider the linearised double shuffle equations, which describe elements of the associated graded of the motivic Lie algebra, with respect to the depth filtration.

In section three, we introduce some of Brown’s motivic machinery: defining motivic multiple zeta values and the motivic coaction. This coaction preserves a filtration - the block filtration - of multiple zeta values, arising from a decomposition due to Charlton. This filtration can be shown to agree with the coradical filtration. We consider the associated graded algebra with respect to this filtration, and attempt to describe all relations in this algebra. The dual Lie algebra is shown to be isomorphic to the motivic Lie algebra, however this block graded Lie algebra has a canonical presentation as a subalgebra of  $\mathbb{Q}\langle e_0, e_1 \rangle$ , suggesting that many of these graded relations should lift to families of relations in among motivic multiple zeta values. In section four, we consider the relationship between the relations satisfied by block graded multiple zeta values, and block graded double shuffle relations.

In section five, we consider the lift of a particular family of block graded relations, soon to appear in work due to Hirose and Sato. We reformulate this in terms of primitivity with respect to a coproduct, and use an explicit isomorphism between the shuffle algebra and the block shuffle algebra to establish yet another family of relations.

Finally, in section six, we consider solutions to the double shuffle equations over fields of finite characteristic, and use this to establish the non-existence of integer and p-adically integral solutions to the shuffle equations. We can then use this to obtain lower bounds on the p-adic valuation of any p-adic or rational solution.

# 1 Drinfel'd Associators and the Geometry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

## 1.1 Multiple zeta values and iterated integrals

The field of study surrounding multiple zeta values is deep, wide and sprawling. One cannot hope to give a comprehensive survey of the current state of affairs within the confines of this thesis, and thus we limit ourselves to a brief overview of the bare necessities. For further details, the author recommends [25] or [33] for a more expository recap.

**Definition 1.1.** For a sequence of integers  $(s_1, \dots, s_r)$  with  $s_i \geq 1$  and  $s_r \geq 2$ , we define the corresponding multiple zeta value by

$$\zeta(s_1, \dots, s_r) := \sum_{0 < n_1 < n_2 < \dots < n_r} \frac{1}{n_1^{s_1} n_2^{s_2} \dots n_r^{s_r}}$$

To a multiple zeta value (often abbreviated MZV), we can associate two quantities: *weight* and *depth*. The weight of  $\zeta(s_1, \dots, s_r)$  is defined to be  $s_1 + s_2 + \dots + s_r$ , and the depth is defined to be  $r$

Let  $\mathcal{Z}$  be the  $\mathbb{Q}$ -vector space  $\mathbb{Q} \oplus \langle \zeta(s_1, \dots, s_r) \rangle_{\mathbb{Q}}$  spanned by multiple zeta values. We can endow this with the structure of an algebra using the *shuffle* relations among MZVs, arising from splitting the summation obtained in the product.

**Example 1.2.**

$$\begin{aligned} \zeta(2)\zeta(3) &= \sum_{m \geq 1} \sum_{n \geq 1} \frac{1}{m^2 n^3} \\ &= \sum_{m < n \leq 1} \frac{1}{m^2 n^3} + \sum_{n < m \leq 1} \frac{1}{m^2 n^3} + \sum_{n \geq 1} \frac{1}{n^5} \\ &= \zeta(2, 3) + \zeta(3, 2) + \zeta(5) \end{aligned}$$

Generalising this example, we see that any product of multiple zeta values lies in  $\mathcal{Z}$ . We make this precise as follows

**Definition 1.3.** Denote a sequence of positive integers  $(i_1, \dots, i_k)$  by the product  $y_{i_1} y_{i_2} \dots y_{i_k}$  in noncommuting formal variables  $y_1, y_2, \dots$ . Denote the empty sequence by 1. Given two sequences of integers,  $y_{i_1} \dots y_{i_r}$  and  $y_{j_1} \dots y_{j_q}$ , we recursively define their stuffle product as the formal sum obtained from

$$\begin{aligned} 1 \star y_{i_1} \dots y_{i_r} &= y_{i_1} \dots y_{i_r} \star 1 = y_{i_1} \dots y_{i_r} \\ y_{i_1} \dots y_{i_r} \star y_{j_1} \dots y_{j_q} &= y_{i_1} (y_{i_2} \dots y_{i_r} \star y_{j_1} \dots y_{j_q}) \\ &\quad + y_{j_1} (y_{i_1} \dots y_{i_r} \star y_{j_2} \dots y_{j_q}) \\ &\quad + y_{i_1+j_1} (y_{i_2} \dots y_{i_r} \star y_{j_2} \dots y_{j_q}) \end{aligned}$$

Then, define  $\zeta(y_{i_1} \dots y_{i_r}) := \zeta(i_1, \dots, i_r)$  and extend  $\zeta$  by linearity to find:

**Proposition 1.4.**

$$\zeta(y_{i_1} \dots y_{i_r}) \zeta(y_{j_1} \dots y_{j_q}) = \zeta(y_{i_1} \dots y_{i_r} \star y_{j_1} \dots y_{j_q})$$

Thus we obtain one algebra structure on MZVs. However, it is not the only such structure. We obtain another product on  $\mathcal{Z}$  by considering the iterated integral representation of MZVs, an idea going back to Chen [11].

**Definition 1.5.** Let  $M$  be a connected differentiable manifold, and let  $\mathcal{P}(M)$  be the set of all paths in  $M$ . To be precise, define

$${}_x\mathcal{P}(M)_y := \{\gamma : [0, 1] \rightarrow M \mid \gamma \text{ piecewise continuous with } \gamma(0) = x, \gamma(1) = y\}$$

and

$$\mathcal{P}(M) := \cup_{x,y \in M} {}_x\mathcal{P}(M)_y$$

Then, given smooth  $k$ -valued 1-forms  $\omega_1, \omega_2, \dots, \omega_r$  on  $M$ , we define the iterated integral of  $\omega_1, \omega_2, \dots, \omega_r$  to be the function

$$\begin{aligned} \int \omega_1, \omega_2, \dots, \omega_r : \mathcal{P}(M) &\rightarrow k \\ \gamma &\mapsto \int_{\gamma} \omega_1 \omega_2, \dots \omega_r \end{aligned}$$

given by

$$\int_{\gamma} \omega_1, \omega_2, \dots, \omega_r = \int_{0 \leq t_1 \leq \dots \leq t_r \leq 1} f_1(t_1) \dots f_r(t_r) dt_1 \dots dt_r$$

where  $f_i(t)dt := \gamma^* \omega_i$ . We view the constant function 1 as an empty iterated integral.

**Remark 1.6.** In this thesis, we perform iterated integrals from left to right. It is equally valid, and quite common to work from right to left. Indeed, it is down to the author's personal preference. Similar differences may be found in the definitions of multiple zeta values. Thus, the reader should not worry if another discussion seems at odds with this one

Multiple zeta values may be obtained as iterated integrals on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  as follows

**Definition 1.7.** Define the 1-form

$$\omega_i := \frac{dz}{z - i}$$

for  $i = 0, 1$ . Then for any binary sequence of the form  $w = 10^{s_1-1}10^{s_2-1}1 \dots 10^{s_r-1}$ , define the differential form

$$\omega_w = \omega_1 \omega_0^{s_1-1} \dots \omega_1 \omega_0^{s_r-1}$$

**Remark 1.8.** Similarly to order of integration in iterated integrals, and order of summation in MZVs, there is no standard convention for these  $\omega_i$ . It is quite common to have this defined as

$$\omega_i := \frac{dz}{i - z}$$

However, the definition given should be consistent with all notions introduced later in this thesis.

**Proposition 1.9.** For a binary sequence of the form  $w = 10^{s_1-1}10^{s_2-1}1 \dots 10^{s_r-1}$ , we obtain upon evaluation of the iterated integral of  $\omega_w$  along the straight line path between 0 and 1

$$\zeta(s_1, \dots, s_r) = (-1)^r \int \omega_w$$

**Remark 1.10.** The reader should note that it is common here to introduce the idea of *tangential basepoints*. While this does not particularly alter the analysis, use of tangential basepoints preserves algebraic information that is necessary in the motivic setting. For more detail, we refer the reader to the work of Deligne [13].

**Example 1.11.** Let  $w := 100$ , then the iterated integral of  $\omega_w$  is given by

$$\begin{aligned}
\int \omega_1 \omega_0 \omega_0 &= \int_0^1 \int_0^x \int_0^y \frac{dz}{z-1} \frac{dy}{y} \frac{dx}{x} \\
&= - \int_0^1 \int_0^x \left( \int_0^y \sum_{i=0}^{\infty} z^i dz \right) \frac{dy}{y} \frac{dx}{x} \\
&= - \int_0^1 \left( \int_0^x \sum_{i=0}^{\infty} \frac{y^i}{i+1} dy \right) \frac{dx}{x} \\
&= - \int_0^1 \sum_{i=0}^{\infty} \frac{x^i}{(i+1)^2} dx \\
&= - \sum_{i=0}^{\infty} \frac{1}{(i+1)^3} = -\zeta(3)
\end{aligned}$$

Now, by considering the product of two multiple zeta values as iterated integrals, and splitting the domain of integration, we obtain another algebra structure on  $\mathcal{Z}$ .

**Example 1.12.**

$$\begin{aligned}
\zeta(2)\zeta(3) &= \int_{0 \leq z \leq y \leq x \leq 1} \frac{dz}{1-z} \frac{dy}{y} \frac{dx}{x} \int_{0 \leq t \leq s \leq 1} \frac{dt}{1-t} \frac{ds}{s} \\
&= \int_{0 \leq z \leq y \leq x \leq t \leq s \leq 1} + \int_{0 \leq z \leq y \leq t \leq x \leq s \leq 1} + \int_{0 \leq z \leq t \leq y \leq x \leq s \leq 1} \\
&+ \int_{0 \leq t \leq z \leq y \leq x \leq s \leq 1} + \int_{0 \leq z \leq y \leq t \leq s \leq x \leq 1} + \int_{0 \leq z \leq t \leq y \leq s \leq x \leq 1} \\
&+ \int_{0 \leq t \leq z \leq y \leq s \leq x \leq 1} + \int_{0 \leq z \leq t \leq s \leq y \leq x \leq 1} + \int_{0 \leq t \leq z \leq s \leq y \leq x \leq 1} \\
&+ \int_{0 \leq t \leq s \leq z \leq y \leq x \leq 1} \frac{dz}{1-z} \frac{dy}{y} \frac{dx}{x} \frac{dt}{1-t} \frac{ds}{s} \\
&= 3\zeta(2, 3) + \zeta(3, 2) + 6\zeta(1, 4)
\end{aligned}$$

To make this precise, we consider  $\zeta$  as a function on  $e_1\mathbb{Q}\langle e_0, e_1 \rangle e_0$ , a sub-vector space of the polynomial algebra in two non-commuting variables as follows:

$$\zeta(e_1 e_0^{s_1-1} e_1 \dots e_1 e_0^{s_r-1}) = \zeta(s_1, \dots, s_r)$$

and extending by linearity. We call monomials in this vector space *convergent words*, and monomials not in this subspace *divergent*.

**Definition 1.13.** Given two elements of  $\mathbb{Q}\langle e_0, e_1 \rangle$ , define their shuffle product recursively by

$$\begin{aligned}
1 \sqcup u &= u \sqcup 1 = u \\
xu \sqcup yv &= x(u \sqcup yv) + y(xu \sqcup v)
\end{aligned}$$

where  $u, v$  are monomials in  $e_0, e_1$ , and  $x, y \in \{e_0, e_1\}$ .

**Proposition 1.14.** For any monomials  $u, v$  in  $e_1\mathbb{Q}\langle e_0, e_1 \rangle e_0$ , we have

$$\zeta(u \sqcup v) = \zeta(u)\zeta(v)$$

Thus we gain a double algebra structure on  $\mathcal{Z}$ , in which we additionally obtain the following relation, arising from the involution of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  that interchanges 0 and 1.

**Proposition 1.15.** *Let  $D : \mathbb{Q}\langle e_0, e_1 \rangle \rightarrow \mathbb{Q}\langle e_0, e_1 \rangle$  be the antihomomorphism mapping  $e_i \mapsto e_{1-i}$ . Then we have  $\zeta(w) = \zeta(Dw)$  for all  $w \in e_1 \mathbb{Q}\langle e_0, e_1 \rangle e_0$ .*

One might feel that restricting ourselves to the sub-vector space  $e_1 \mathbb{Q}\langle e_0, e_1 \rangle e_0$  is quite limiting, and this is to some extent true. Fortunately, there exist regularisation procedures, one compatible with the shuffle algebra structure and one compatible with the stuffle algebra structure, which allow us to extend  $\zeta$  to a function on all of  $\mathbb{Q}\langle e_0, e_1 \rangle$  [27]. Indeed, these regularised MZVs prove critical in providing sufficient relations for conjectured dimensions of the various weight spaces of  $\mathcal{Z}$  to hold.

We now mention a few standard conjectures in the theory of MZVs.

**Conjecture 1.16.**  $\mathcal{Z}$  is weight graded: defining  $\mathcal{Z}_n := \langle \zeta(s_1, \dots, s_r) | s_1 + \dots + s_r = n \rangle_{\mathbb{Q}}$ , we have

$$\mathcal{Z} = \bigoplus_{n=0}^{\infty} \mathcal{Z}_n$$

where we take  $\zeta(\emptyset) = 1$ .

**Conjecture 1.17.** The weight graded pieces of  $\mathcal{Z}$  have dimensions given by the generating series

$$\sum_{n=0}^{\infty} \dim \mathcal{Z}_n t^n = \frac{1}{1 - t^2 - t^3}$$

**Conjecture 1.18.** All relations among multiple zeta values can be obtained from the shuffle and stuffle relations, alongside the Hoffman relation:

$$\zeta(e_1 \sqcup u - e_1 \star u) = 0$$

for all convergent  $u$ .

## 1.2 Drinfel'd associators and the KZ equations

In his 1990 work [15] Drinfel'd introduced the idea of an *associator*, a power series in two non-commuting variables.

**Definition 1.19.** Let  $k$  be a field of characteristic 0 and  $\lambda \neq 0 \in k$ . A  $\lambda$ -*associator* over a  $k$  is an element  $\Phi \in k\langle\langle e_0, e_1 \rangle\rangle$  that is grouplike for the continuous coproduct

$$\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i$$

and satisfies the pentagon and hexagon equations

$$\Phi(t_{12}, t_{23} + t_{24})\Phi(t_{13} + t_{23}, t_{34}) = \Phi(t_{23}, t_{34})\Phi(t_{12} + t_{13}, t_{24} + t_{34})\Phi(t_{12}, t_{23})$$

$$\exp\left(\frac{\pm \lambda e_0}{2}\right)\Phi(e_{\infty}, e_0)\exp\left(\pm \frac{\lambda e_{\infty}}{2}\right)\Phi(e_1, e_{\infty})\exp\left(\pm \frac{\lambda e_1}{2}\right)\Phi(e_0, e_1) = 1$$

where  $e_{\infty} = -e_0 - e_1$  and the  $t_{ij}$  are the infinitesimal braid variables, satisfying the following:

$$\begin{aligned} t_{ii} &= 0 \\ t_{ij} &= t_{ji} \\ [t_{ij}, t_{kl}] &= 0 \text{ if } i, j, k, l \text{ distinct} \\ [t_{ij}, t_{ik} + t_{jk}] &= 0 \text{ if } i, j, k \text{ distinct} \end{aligned}$$

Together, we refer to these equations as the associator equations.

Interestingly, the hexagon equations are, to some extent, unnecessary, as shown by Furusho [18].

**Theorem 1.20** (Furusho). *Let  $\Phi$  be a grouplike power series in two non commuting variables, satisfying Drinfel'd's pentagon equation. Then there is a unique  $\lambda$ , depending only on the coefficient of the degree 2 terms, such that the pair  $(\lambda, \Phi)$  satisfy the hexagon equations.*

While arising originally from the study of quasi-Hopf algebras and braided monoidal categories, associators have since sparked interest in many areas of mathematics, including knot invariants [2], quantum field theory and deformation-quantisation[28], and number theory. In particular, the ties between associators and the Grothendieck-Teichmüller group has drawn much interest.

The Grothendieck-Teichmüller group is quite an important object in algebra, acting on a range of objects in various fields. It exists in three versions: a profinite version, a pro- $l$  version and a pro-unipotent version. The first two are of interest, as the action of the absolute Galois group factors through them, while the latter arises in homological algebra and motivic contexts. It is this last version that appears in the discussion of associators.

**Definition 1.21.** Define the Grothendieck-Teichmüller group  $GT$  to be the affine group scheme over  $\mathbb{Q}$ , whose  $k$  points are given by pairs  $(\lambda, f)$  in  $k^\times \times k\langle\langle x, y \rangle\rangle$  such that

$$\begin{aligned}\Delta f &= f \hat{\otimes} f \\ f(y, x) &= f(x, y)^{-1} \\ f(z, x)z^{\frac{\lambda-1}{2}}f(y, z)y^{\frac{\lambda-1}{2}}f(x, y)x^{\frac{\lambda-1}{2}} &= 1 \\ f(x_{12}, x_{23}x_{24})f(x_{13}x_{23}, x_{34}) &= f(x_{23}, x_{34})f(x_{12}x_{13}, x_{24}x_{34})f(x_{12}, x_{23})\end{aligned}$$

where  $xyz = 1$  and  $x_{ij}$  are elements of the pure braid group, and  $\Delta$  is the completed coproduct for which  $x, y$  are primitive. We endow this with a group structure as follows

$$(\lambda, f) \cdot (\lambda', f')(x, y) = (\lambda\lambda', f(x, y)f'(x^\lambda, f^{-1}y^\lambda f))$$

**Remark 1.22.** The coefficient of  $e_0e_1$  in  $f$  nearly determines  $\lambda$ . To be precise, the coefficient is  $\frac{\lambda^2}{24}$ .

$GT$  acts on the space of associators on the left. We get a similar action on the right by the space of ‘0-associators’, which we call the graded Grothendieck-Teichmüller group  $GRT$ . To be precise  $GRT_1$  is the space of power series  $\Phi \in k\langle\langle e_0, e_1 \rangle\rangle$  solving the equations of Definition 1.19 with  $\lambda = 0$ , and  $GRT := k^\times \ltimes GRT_1$  with  $\mu \cdot \Phi(e_0, e_1) := \Phi(\mu e_0, \mu e_1)$ , with product defined by

$$\Phi \cdot \Phi'(e_0, e_1) := \Phi'(e_0, e_1)\Phi(e_0, \Phi'^{-1}e_1\Phi')$$

One can show [15] that the space of associators is a  $GT$ - $GRT$  torsor, and hence  $GT \cong GRT$ . Thus, by studying associators, in particular 0-associators, we can gain information about  $GT$ .

One of the first questions one might have about the space of associators is whether it is empty? It is far from obvious that a solution to the associator equations exists for any  $\lambda$ . Drinfel'd in fact showed a solution existed and constructed it explicitly [15] from the monodromy of the Knizhnik Zamolodchikov equations.

**Theorem 1.23** (Drinfel'd). *There exists a solution to the associator equations whose coefficients are given by multiple zeta values*

$$\Phi(e_0, e_1) = \sum_{w \in \langle e_0, e_1 \rangle} (-1)^{|w|} \zeta(w) w$$

This adds a further layer of number theoretical interest to the problem of associators, as multiple zeta values are now constrained by the associator equations, giving relations between them. It is in fact conjectured that they describe all non trivial relations between multiple zeta values. However, the associator equations are notoriously challenging, and so the following corollary becomes tremendously useful in describing potential relations among multiple zeta values.

**Corollary 1.24.** *There exists an associator with coefficients in  $\mathbb{Q}$ .*

We will only give the barest of sketches of a proof of this corollary. Should the reader be interested, we recommend either Drinfel'd original work [15], or, if the reader is comfortable with braid theoretic language, Bar-Natan's constructive proof [2].

**Sketch.** It is known that  $\text{GRT} \cong \mathbb{G}_m \rtimes U$ , for  $U$  a pronipotent group. Hence, GRT has trivial Galois cohomology, and any torsor over GRT must also be trivial. Thus, if the space of associators is non-empty over any field containing  $\mathbb{Q}$ , it is non empty over  $\mathbb{Q}$ . We have a  $\mathbb{C}$ -associator, and therefore there exist  $\mathbb{Q}$ -associators.

We also sketch the proof of the theorem, based on the discussion of [31].

**Definition 1.25.** The Knizhnik Zamolodchikov equations are a system of differential equations

$$\frac{\partial \psi}{\partial x_i} = \sum_{j \neq i} \frac{t_{ij}}{x_i - x_j} \psi$$

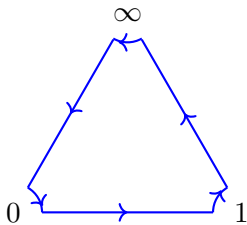
where  $t_{ij}$  are defined as above.

**Sketch.** The connection on  $\mathcal{M}_{0,4}$  arising from the KZ equations is given by

$$\nabla = d - t_{12} \frac{dz}{z} - t_{23} \frac{dz}{z-1}$$

Define  $\Phi(t_{12}, t_{23})$  to be the holonomy of this connection from  $z = 0$  to  $z = 1$ . We again should consider tangential basepoints here, but we shall gloss over this technicality. Using standard techniques, we compute the holonomy to be

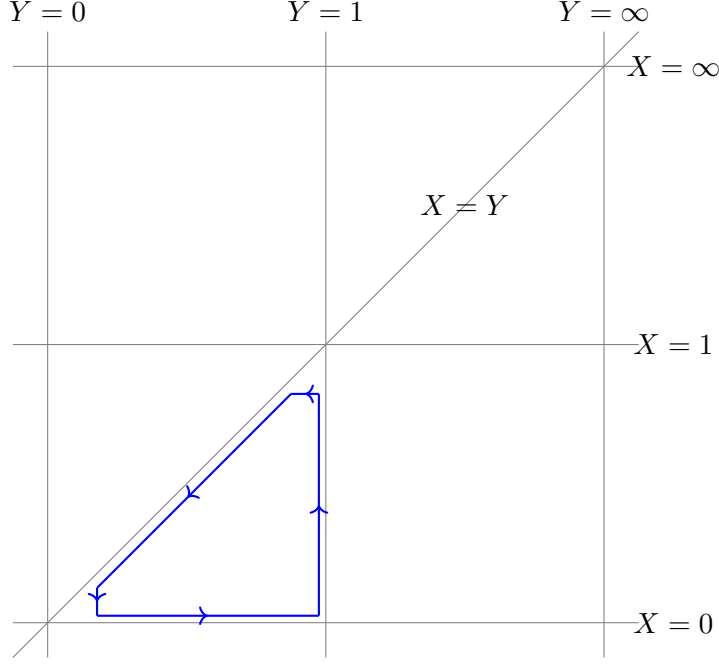
$$\begin{aligned} \Phi(t_{12}, t_{13}) = & \lim_{t \rightarrow 0} t^{-t_{23}} \left( 1 + \int_0^1 t_{12} \frac{dt_1}{t_1} + t_{23} \frac{dt_1}{t_1 - 1} + \dots \right. \\ & \left. + \int_{0 \leq t_1 \leq \dots \leq t_n \leq 1} (t_{12} \frac{dt_1}{t_1} + t_{23} \frac{dt_1}{t_1 - 1}) (\dots) (t_{12} \frac{dt_n}{t_n} + t_{23} \frac{dt_n}{t_n - 1}) + \dots \right) t^{t_{12}} \end{aligned}$$



To see that this solves the associator equations, we simply consider the holonomy along various paths. For example, the hexagon equations follows from computing the holonomy along the illustrated cycle.

The pentagon equation follows similarly, by integration along a closed curve in  $\mathcal{M}_{0,5}$ , illustrated below. Then explicitly calculating the integrals gives our result.

This project begins in searching for an explicit canonical rational associator. We know that they exist, but none are known explicitly. We even have iterative constructions for rational solutions to the associator equations up to a given weight. However, these constructions involves many choices, and are unlikely to give an explicit formula for the coefficients. As such, we consider alternative approaches: looking more generally at relations among multiple zeta values defined over the rationals, and seeing if they can be used to impose canonical conditions.



### 1.3 The double shuffle equations

The first obstruction to finding a rational associator is the difficulty in finding any associator. Thus we will instead attempt to solve a simpler problem: solving the double shuffle equations. We know multiple zeta values satisfy a set of shuffle relations, and we expect the associator equations to imply all relations among multiple zeta values. Thus it makes sense to model our easier equations on known MZV relations. In the following definitions, due to Racinet [30], let  $k$  be a field. It need not be of characteristic zero, but is normally taken to be.

**Definition 1.26.** We say a power series  $\Phi \in k\langle\langle a, b \rangle\rangle$  solves the shuffle equations if it is grouplike for the completed coproduct for which  $a, b$  are primitive. That is

$$\Delta\Phi = \Phi \otimes \Phi$$

where

$$\Delta(x) = x \otimes 1 + 1 \otimes x \text{ for } x = a, b$$

**Definition 1.27.** Let  $Y = y_1, y_2, y_3, \dots$  be a collection of formal variables. We say a power series  $\Phi \in k\langle\langle Y \rangle\rangle$  solves the stuffle equations if it is grouplike for the completed coproduct, defined on generators by

$$\Delta_*(y_n) = \sum_{i=0}^n y_i \otimes y_{n-i}$$

where we define  $y_0 := 1$ .

**Definition 1.28.** Define the projection map  $\pi_Y : k\langle\langle a, b \rangle\rangle \rightarrow k\langle\langle Y \rangle\rangle$  to be the linear map given by

$$\pi_Y(ba^{n_1-1}ba^{n_2-1}\dots ba^{n_k-1}) = y_{n_1}y_{n_2}\dots y_{n_k}$$

and  $\pi_Y(aw) = 0$  for any word  $w \in k\langle a, b \rangle$ . Define also, for any element  $\Phi \in k\langle\langle a, b \rangle\rangle$ ,  $\Phi_{corr} \in k\langle\langle Y \rangle\rangle$  by

$$\Phi_{corr} := \exp\left(\sum_{n \geq 1} \frac{(-1)^n}{n} (\Phi|ba^{n-1})y_1^n\right)$$

where  $(\Phi|w)$  denotes the coefficient of  $w$  in  $\Phi$ .

**Definition 1.29.** We say a power series  $\Phi \in k\langle\langle a, b \rangle\rangle$  solves the (regularised) double shuffle equations if  $\Phi$  solves the shuffle equations and  $\Phi^* := \Phi_{\text{corr}} \pi_Y(\Phi)$  solves the stuffle equations.

While still challenging to solve, the double shuffle equations are much more tractable, and allow us to make use of additional structures coming from MZVs, such as the depth and weight filtrations. While both the double shuffle equations and the associator equations are weight graded, describing the weight graded pieces of the double shuffle equations is much easier than those of the associator equations. We can split the double shuffle equations into depth filtered pieces, but there is no clear analogue of depth in the pentagon equation. Furthermore, it is commonly conjectured that the double shuffle equations describe all possible relations among MZVs, and are hence equivalent to the associator equations. However, little is known about this beyond the work of Furusho [19].

**Theorem 1.30.** *Let  $\Phi$  be a grouplike power series in two noncommuting variable. Suppose also that it satisfies the pentagon equation. Then  $\Phi$  solves the double shuffle equations.*

The space of solutions to the double shuffle equations, denoted  $\text{DMR}$ , contains a subspace of solutions,  $\text{DMR}_0$ , such that  $(\Phi|_{e_0}) = (\Phi|_{e_1}) = (\Phi|_{e_0 e_1}) = 0$ . This subspace forms a pro-unipotent group [30] with multiplication given by

$$\Phi \cdot \Phi'(e_0, e_1) := \Phi'(e_0, e_1) \Phi(e_0, \Phi'^{-1} e_1 \Phi')$$

which the reader will note is identical to that of  $GRT$ . Thus we get the following

**Corollary 1.31.**  *$GRT$  is a subgroup of  $\text{DMR}_0$*

It is a standard conjecture that they are in fact equal to the unipotent part of the motivic Galois group, which we shall later discuss in greater depth.

Looking to the shuffle equations has proven quite fruitful, as they also lend themselves well to a rewriting in terms of commutative power series. a technique due to Brown, and very similar to Écalle's theory of moulds [16], this technique has allowed Brown to define a canonical rational associator up to depth 4.

**Remark 1.32.** From this point in the text, we are interested only in  $\text{DMR}_0$ , and so we shall assume  $(\Phi|_{e_0}) = (\Phi|_{e_1}) = (\Phi|_{e_0 e_1}) = 0$  for all potential solutions to the shuffle or stuffle equations.

**Definition 1.33.** Denote by  $D_n$  the vector space spanned by words of depth  $n$  in  $k\langle a, b \rangle$  and let  $\rho_n : D_n \rightarrow k[[y_0, y_1, \dots, y_n]]$  be the isomorphism of vector spaces given by

$$\rho_n(a^{m_0} b a^{m_1} b \dots b a^{m_n}) = y_0^{m_0} y_1^{m_1} \dots y_n^{m_n}$$

The map  $\rho := \sum_{n=1}^{\infty} \rho_n$ , then defines an isomorphism

$$\begin{aligned} \rho : k\langle a, b \rangle &\rightarrow \bigoplus_{n=1}^{\infty} k[y_0, \dots, y_n] \\ \Phi &\mapsto \{\Phi^{(n)}(y_0, \dots, y_n)\}_{n=1}^{\infty} \end{aligned}$$

We can then define the double shuffle equations in this new formulation as polynomial equations.

First we note the following lemma.

**Lemma 1.34.** *If  $\Phi = 1 + \Phi_1 + \Phi_2 + \dots$  solves the shuffle equations, where  $\Phi_n$  is the depth  $n$  component of  $\Phi$ , then  $\rho_n(\Phi_n) \in k[y_0, \dots, y_n]$  is translation invariant.*

*Proof.* Define  $\delta : k\langle a, b \rangle \rightarrow k\langle a, b \rangle$  to be the derivation given on generators by

$$\begin{aligned}\delta(a) &:= 1 \\ \delta(b) &:= 0\end{aligned}$$

Note that

$$\delta(a^{m_0}ba^{m_1}b \dots ba^{m_k}) = \sum_{i=0}^k m_i a^{m_0}ba^{m_1}b \dots ba^{m_i-1}b \dots ba^{m_k}$$

and that this agrees with the derivation given by  $(\pi_0 \otimes id) \circ \Delta$ , where  $\pi_0(\Phi) := (\Phi|e_0)$ . Thus, if  $\Delta\Phi = \Phi \otimes \Phi$ , we get

$$\delta\Phi = (\Phi|e_0)\Phi = 0$$

But since  $\delta$  preserves depth, this clearly implies  $\delta\Phi_n = 0$ . Translating into the language of commutative power series, we get

$$\sum_{i=0}^n \frac{\partial}{\partial y_i} \Phi^{(n)} = 0$$

□

In light of this, we lose no information about solutions to the double shuffle equations by setting  $y_0 = 0$ . Indeed, this is how we shall proceed. In a slight abuse of notation, we shall still refer to the resulting polynomial as  $\Phi^{(n)}$ . In order to make our discussion unambiguous, we shall adopt the following notational distinction.

$$\begin{aligned}\Phi^{(n)}(y_0, y_1, \dots, y_n) &:= \rho_n(\Phi_n)(y_0, \dots, y_n) \\ \Phi^{(n)}(x_1, \dots, x_n) &:= \rho_n(\Phi_n)(0, x_1, \dots, x_n)\end{aligned}$$

That is, we will use  $y_i$  as variables for the image of  $\rho$ , and  $x_i$  as variables for the power series obtained by setting  $y_0 = 0$ . We can now define the double shuffle equations in the language of commutative power series.

**Definition 1.35.** Given a polynomial  $f \in k[x_1, \dots, x_n]$ , define  $f^\# \in k[x_1, \dots, x_n]$  by

$$f^\#(x_1, \dots, x_n) := f(x_1, x_1 + x_2, x_1 + x_2 + x_3, \dots, x_1 + x_2 + \dots + x_n)$$

We also define recursively the polynomial

$$\begin{aligned}f(\mathbf{x}_1 \dots \mathbf{x}_j \sqcup \mathbf{x}_{j+1} \dots \mathbf{x}_n) &:= \\ f(\mathbf{x}_1, (\mathbf{x}_2 \dots \mathbf{x}_j \sqcup \mathbf{x}_{j+1} \dots \mathbf{x}_n) &+ f(\mathbf{x}_{j+1}, (\mathbf{x}_1 \dots \mathbf{x}_j \sqcup \mathbf{x}_{j+2} \dots \mathbf{x}_n)\end{aligned}$$

where  $f(\mathbf{x}_1 \dots \mathbf{x}_n) := f(x_1, \dots, x_n)$ .

**Definition 1.36.** We say a family of polynomials  $\{f^{(n)}\}$  solves the shuffle equations if

$$f^{(n)\#}(\mathbf{x}_1 \dots \mathbf{x}_j \sqcup \mathbf{x}_{j+1} \dots \mathbf{x}_n) = f^{(j)}(x_1, \dots, x_j) f^{(n-j)}(x_{j+1}, \dots, x_n)$$

for all  $1 \leq j < n$ .

Defining the stuffle equations is slightly more challenging and requires a few extra definitions

**Definition 1.37.** For any family of polynomials  $\{f^{(n)}\}$ , define the operators

$$s_i f^{(r)}(x_1, \dots, x_r) := f^{(r+1)}(x_i, x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_r) \text{ for } 1 \leq i \leq r$$

**Definition 1.38.** Define recursively

$$\begin{aligned} f^{(r)}(1 \star x_1 \dots x_r) &= f^{(r)}(x_1 \dots x_r \star 1) = f^{(r)}(x_1, \dots, x_r) \\ f^{(r)}(x_1 \dots x_i \star x_{i+1} \dots x_r) &= s_1 f^{(r-1)}(x_2 \dots x_i \star x_{i+1} \dots x_r) \\ &\quad + s_{i+1} f^{(r-1)}(x_1 \dots x_i \star x_{i+2} \dots x_r) \\ &\quad + \left( \frac{s_1 - s_{i+1}}{x_1 - x_{i+1}} \right) f^{(r-2)}(x_2 \dots x_i \star x_{i+2} \dots x_r) \end{aligned}$$

where  $1 \leq i \leq r$ .

**Definition 1.39.** We say a family of polynomials  $\{f^{(n)}\}$  solves the stuffle equations if

$$f^{(n)}(x_1 \dots x_j \star x_{j+1} \dots x_n) = f^{(j)}(x_1, \dots, x_j) f^{(n-j)}(x_{j+1}, \dots, x_n)$$

for all  $1 \leq j < n$ .

**Remark 1.40.** Note that in this formulation, there is no mention of an analogue to  $\Phi_{corr}$ . While it is true that we must add a corresponding correction term, we shall ignore this for sake of this discussion. However, we will ask the reader to observe that this arises naturally for multiple zeta values, by considering shuffle regularisation versus stuffle regularisation.

**Example 1.41.** In depth 2, the double shuffle equations are

$$\begin{aligned} f^{(2)}(x_1, x_1 + x_2) + f^{(2)}(x_2, x_1 + x_2) &= f^{(1)}(x_1) f^{(1)}(x_2) \\ f^{(2)}(x_1, x_2) + f^{(2)}(x_1, x_2) + \frac{f^{(1)}(x_1) - f^{(1)}(x_2)}{x_1 - x_2} &= f^{(1)}(x_1) f^{(1)}(x_2) \end{aligned}$$

while in depth 3, they become

$$\begin{aligned} f^{(3)}(x_1, x_1 + x_2, x_1 + x_2 + x_3) + f^{(3)}(x_2, x_1 + x_2, x_1 + x_2 + x_3) + f^{(3)}(x_2, x_2 + x_3, x_1 + x_2 + x_3) \\ = f^{(1)}(x_1) f^{(2)}(x_2, x_3) \\ f^{(3)}(x_1, x_2, x_3) + f^{(3)}(x_2, x_1, x_3) + f^{(3)}(x_2, x_3, x_1) + \frac{f^{(2)}(x_1, x_3) - f^{(2)}(x_2, x_3)}{x_1 - x_2} + \frac{f^{(2)}(x_2, x_1) - f^{(2)}(x_2, x_3)}{x_1 - x_3} \\ = f^{(1)}(x_1) f^{(2)}(x_2, x_3) \end{aligned}$$

**Remark 1.42.** From this point onward, we shall often neglect the superscript  $f^{(n)}$ , instead writing only  $f$ , as it should be obvious from the number of variables to which depth we refer.

## 1.4 The motivic Galois group and the geometry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

With such impressive symmetries amongst MZVs, one might hope for some sort of transcendental Galois theory. This is to some extent found in the *motivic* Galois group associated to a certain Tannakian category associated to  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . As general references, the works of Ayoub [1], Deligne [12] and Brown [6],[5] can be useful.

Let  $\mathcal{MT}(\mathbb{Z})$  denote the category of mixed Tate motives unramified over  $\mathbb{Z}$ . This is a Tannakian category, and hence is equivalent to the category of representations of a group scheme, called its Galois group and denoted by  $G_{\mathcal{MT}(\mathbb{Z})}$ .  $\mathcal{MT}(\mathbb{Z})$  contains as a full Tannakian subcategory  $\mathcal{MT}'(\mathbb{Z})$ , the Tannakian subcategory generated by the motivic fundamental group of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . We hence obtain a map

$$G_{\mathcal{MT}(\mathbb{Z})} \rightarrow G_{\mathcal{MT}'(\mathbb{Z})}$$

We now define the motivic fundamental group of  $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ , or rather, the motivic fundamental groupoid, of which the motivic fundamental group is a special case.

**Definition 1.43.** Let  $x, y$  be points of  $X(\mathbb{C})$ . The motivic fundamental groupoid of  $X$  consists of the following

- (Betti) A collection of schemes  $\pi_1^B(X, x, y)$  defined over  $\mathbb{Q}$  and equipped with the structure of a groupoid

$$\pi_1^B(X, x, y) \times \pi_1^B(X, y, z) \rightarrow \pi_1^B(X, x, z)$$

for any  $x, y, z \in X(\mathbb{C})$ . There is a natural homomorphism

$$\pi_1^{top}(X, x, y) \rightarrow \pi_1^B(X, x, y)(\mathbb{Q})$$

where the fundamental groupoid on the left is given by the homotopy classes of paths relative to their endpoints.

- (de Rham) An affine group scheme over  $\mathbb{Q}$ , denoted by  $\pi_1^{dR}(X)$ .
- (Comparison) A canonical isomorphism of schemes over  $\mathbb{C}$

$$\text{comp} : \pi_1^B(X, x, y) \times_{\mathbb{Q}} \mathbb{C} \rightarrow \pi_1^{dR}(X) \times_{\mathbb{Q}} \mathbb{C}$$

**Remark 1.44.** We once again gloss over the technicalities of tangential basepoints. For sake of precision, the reader should read  $\pi_1^\bullet(X, 0, 1)$  as  $\pi_1^\bullet(X, \vec{1}_0, -\vec{1}_1)$  where  $\vec{1}_x$  denotes the unit vector parallel to the real line, based at  $x$ . Thus, all paths  $\gamma : (0, 1) \rightarrow \mathbb{C} \setminus \{0, 1\}$  with  $\gamma(0) = 0$ ,  $\gamma(1) = 1$  in the following discussion have  $\gamma'(0) = \gamma'(1) = 1$ .

**Theorem 1.45.** *There is an ind-object*

$$\mathcal{O}(\pi_1^{mot}(X, 0, 1)) \in \text{Ind}(\mathcal{MT}(\mathbb{Z}))$$

whose Betti and de Rham realisations are the affine rings  $\mathcal{O}(\pi_1^B(X, 0, 1))$  and  $\mathcal{O}(\pi_1^{dR}(X))$  respectively.

Define  ${}_0\Pi_1 := \text{Spec}(\mathcal{O}(\pi_1^{dR}(X)))$ . This is the affine scheme over  $\mathbb{Q}$  which associates to any commutative unitary  $\mathbb{Q}$ -algebra  $R$  the set of grouplike formal power series

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

where  $\Delta$  is the completed coproduct for which  $e_i$  are primitive.

This carries an action of the motivic Galois group  $G_{\mathcal{MT}(\mathbb{Z})}^{dR}$ , which depends on our choice of basepoints, even though  $\pi_1^{dR}(X)$  does not contain an explicit dependence on these points.

**Remark 1.46.** Among all paths in  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  from 0 to 1 satisfying our velocity constraints, there is a distinguished straight line path  $\gamma(t) = t$ , referred to as the *droit chemin* and denoted *dch*. The natural homomorphism mentioned in Definitions 1.43 maps *dch* onto an element  ${}_0 1_1^B \in \pi_1^B(X, 0, 1)(\mathbb{Q})$ . The image of this map under the comparison isomorphism is precisely the Drinfel'd associator

$$\text{comp}({}_0 1_1^B) = \sum_w \zeta(w) w \in {}_0\Pi_1(\mathbb{C})$$

The action of  $G_{\mathcal{MT}(\mathbb{Z})}$  is made more transparent via the decomposition

$$G_{\mathcal{MT}(\mathbb{Z})} = U_{\mathcal{MT}(\mathbb{Z})} \rtimes \mathbb{G}_m$$

into a semidirect product of a pro-unipotent  $U_{\mathcal{MT}(\mathbb{Z})}$  and the multiplicative group.

The action of  $G_{\mathcal{MT}(\mathbb{Z})}$  restricts to an action

$$U_{\mathcal{MT}(\mathbb{Z})} \times {}_0\Pi_1 \rightarrow {}_0\Pi_1$$

which factors through a map

$$\circ^* : {}_0\Pi_1 \times {}_0\Pi_1 \rightarrow {}_0\Pi_1$$

called the Ihara action, computed explicitly first by Y. Ihara, but described in [12].

**Remark 1.47.** We later introduce the *linearised*, or *infinitesimal* Ihara action, in the context of the Lie algebras of  $\mathrm{DMR}_0$  and  $U_{\mathcal{MT}(\mathbb{Z})}$ . The reader must take care to avoid confusing the two.

## 2 Double Shuffle Modulo Products and Canonical Generators

### 2.1 The double shuffle Lie algebra

In order to further simplify the equations, we can move from  $\text{DMR}_0$  to its Lie algebra  $\mathfrak{dmr}_0$ , and consider solutions to the double shuffle equations *mod products*.

**Definition 2.1.** We say  $\sigma \in k\langle a, b \rangle$  solves the double shuffle equations mod products if the following hold

$$\begin{aligned}\Delta\sigma &= \sigma \otimes 1 + 1 \otimes \sigma \\ \Delta_*(\sigma^*) &= \sigma^* \otimes 1 + 1 \otimes \sigma^* \\ (\sigma|a) &= (\sigma|b) = (\sigma|ab) = 0\end{aligned}$$

where  $\sigma^* := \pi_Y \sigma + \sigma_{\text{corr}}$ , where  $\sigma_{\text{corr}} := \sum_{n \geq 1} \frac{(-1)^n}{n} (\sigma|ba^{n-1}) y_1^n$ .

Note that the double shuffle equations mod products are homogeneous for weight, and thus we will often assume all monomials in  $\sigma$  to be of the same weight, allowing us to refer to solutions of a particular weight.

Once again, we can rephrase this in terms of commutative variables. We first note the following lemma

**Lemma 2.2** (Brown). *If  $\sigma$  solves the shuffle equations, i.e.  $\sigma$  is primitive, then  $\rho(\sigma)$  is translation invariant, where  $\rho$  is as defined previously.*

**Definition 2.3.** We say  $\{f_j \in k[x_1, \dots, x_j]\}_{j=1}^n$  solves the shuffle equations mod products up to depth  $n+1$  if

$$f_j^\#(\mathbf{x}_1 \dots \mathbf{x}_i \sqcup \mathbf{x}_{i+1} \dots \mathbf{x}_j) = 0$$

for all  $1 \leq i < j \leq n$ . We say  $\{f_j \in k[x_1, \dots, x_j]\}_{j=1}^n$  solves the stuffle equations mod products up to depth  $n+1$  if

$$f_j(\mathbf{x}_1 \dots \mathbf{x}_i \star \mathbf{x}_{i+1} \dots \mathbf{x}_j) = 0$$

for all  $1 \leq i < j \leq n$ .

We once again should consider correction terms in the stuffle equations in order to say  $f$  solves the double shuffle equations mod products. However, as we may assume  $f$  is homogeneous in weight, the correction terms arise only in the depth-equal-to-weight equations, and are easily accounted for. Thus, we say a family of polynomials  $\{f_i \in k[x_1, \dots, x_i]\}_{i=1}^n$  is a solution of weight  $n+1$  to the double shuffle equations mod products if it solves the shuffle and stuffle equations mod products up to depth  $n+1$ .

We now define the Lie algebra structure, which arises via derivations [30] or from the anti-symmetrisation of the Ihara action [7].

**Definition 2.4.** Given  $\psi \in k\langle a, b \rangle$ , define the derivation  $d_\psi : k\langle a, b \rangle \rightarrow k\langle a, b \rangle$  by

$$\begin{aligned}d_\psi(a) &= 0 \\ d_\psi(b) &= [b, \psi]\end{aligned}$$

We define the Ihara bracket  $\{\cdot, \cdot\} \wedge^2 k\langle a, b \rangle \rightarrow k\langle a, b \rangle$  by

$$\{\sigma_1, \sigma_2\} := d_{\sigma_2} \sigma_1 - d_{\sigma_1} \sigma_2 - [\sigma_1, \sigma_2]$$

Alternatively, we can define:

**Definition 2.5.** Define the linearised Ihara action  $\circ : k\langle a, b \rangle \otimes k\langle a, b \rangle \rightarrow k\langle a, b \rangle$  by

$$u \circ a^n bv := a^n ubv + a^n bu^*v + a^n b(u \circ v)$$

where, if  $u = u_1 u_2 \dots u_r$ ,  $u^* = (-1)^r u_r \dots u_1$  and  $u \circ a^n = a^n u$ , for all  $u, v$  monomials in  $k\langle a, b \rangle$ , and extend linearly. Define the Ihara bracket by

$$\{\sigma_1, \sigma_2\} = \sigma_1 \circ \sigma_2 - \sigma_2 \circ \sigma_1$$

We then obtain the following from Racinet's thesis.

**Proposition 2.6** (Racinet).  *$\mathfrak{d}\mathfrak{mr}_0$  equipped with the Ihara bracket is a Lie algebra. Furthermore, the function*

$$\exp_{\circ}(\sigma) := 1 + \sigma + \frac{1}{2}\sigma \circ \sigma + \frac{1}{6}\sigma \circ \sigma \circ \sigma + \dots$$

*defines a map  $\exp_{\circ} : \mathfrak{d}\mathfrak{mr}_0 \rightarrow DMR_0$ .*

The Ihara action, and hence the Ihara bracket are motivic: they arise naturally from the group structure of  $U_{\mathcal{MT}(\mathbb{Z})}$ . In fact, one can show  $\mathfrak{g}^{\mathfrak{m}} := \text{Lie}(U_{\mathcal{MT}(\mathbb{Z})}) \subset \mathfrak{d}\mathfrak{mr}_0$  [19], thus the study of  $\mathfrak{d}\mathfrak{mr}_0$  gives us information about both associators and the motivic Galois group. This inclusion is conjecturally an isomorphism of Lie algebras, which gives us a method of generating solutions to the double shuffle equations: we have the non-canonical isomorphism

$$\mathfrak{g}^{\mathfrak{m}} \cong \mathbb{L}(\sigma_3, \sigma_5, \dots)$$

to the free Lie algebra with a generator in every odd degree greater than 1. Thus, given the  $\sigma_{2n+1}$ , we can produce solutions to the double shuffle equations in any weight. However, the isomorphism is not canonical, nor do we have a canonical representation of these  $\sigma_{2k+1}$  in  $\mathbb{Q}\langle e_0, e_1 \rangle$ . We have that

$$\sigma_{2n+1} = \text{ad}^{2n}(a)(b) + \text{terms of higher depth}$$

where the adjoint action is with respect to the Lie bracket  $[X, Y] = XY - YX$ . However, the double shuffle equations give us no power to distinguish between  $\sigma_{2n+1}$  and  $\sigma_{2n+1} + \phi$  where  $\phi \in \mathfrak{d}\mathfrak{mr}_0$  is of depth at least 2. Thus the  $\sigma_{2n+1}$  are ambiguous up to brackets of lower weight elements of  $\mathfrak{g}$ , limiting their computational use.

## 2.2 Canonical elements and polar solutions

The first thing one might desire is to make the  $\sigma$ -elements canonical, to have an explicit generating set. There seem to be three main approaches to doing so: using inner products and a Gram-Schmidt-like procedure, using a basis of multiple zeta values, or Brown's anatomical decomposition. The first approach has not been seen in the literature to this point, and so we focus on this, finding several new results.

**Theorem 2.7** (Keilthy, Hain). *Given a choice of inner product on  $\mathbb{Q}\langle e_0, e_1 \rangle$ , we can define a unique embedding of  $\{\sigma_3, \sigma_5, \sigma_7, \dots\} \hookrightarrow \mathbb{Q}\langle e_0, e_1 \rangle$ , and hence of the motivic Lie algebra.*

*Proof.* Suppose that we have a fixed embedding of  $\sigma_3, \dots, \sigma_{2k-1}$  into  $\mathbb{Q}\langle e_0, e_1 \rangle$  and consider the space  $\mathbb{L}(\sigma_3, \dots, \sigma_{2k+1})_{2k+1}$ , where the subscript denotes the sub-vector space spanned by elements of weight  $2k+1$ . This contains  $\mathbb{L}(\sigma_3, \dots, \sigma_{2k-1})_{2k+1}$  as a codimension 1 subspace, and thus, given a non-degenerate inner product, we can fix  $\sigma_{2k+1}$  up to a scalar multiple by imposing orthogonality of  $\sigma_{2k+1}$  to  $\mathbb{L}(\sigma_3, \dots, \sigma_{2k-1})_{2k+1}$ . Thus, as  $\sigma_3$  has a unique embedding into  $\mathbb{Q}\langle e_0, e_1 \rangle$ , given an inner product, we can define a unique embedding of every  $\sigma_{2k+1}$ .  $\square$

There are two natural candidates for our inner product  $\langle \cdot, \cdot \rangle : \mathbb{Q}\langle a, b \rangle \times \mathbb{Q}\langle a, b \rangle \rightarrow \mathbb{Q}$ . Define for monic monomials  $u, v$

$$\begin{aligned}\langle u, v \rangle_{triv} &:= \begin{cases} 1 & \text{if } u = v \\ 0, & \text{otherwise} \end{cases} \\ \langle u, v \rangle_S &:= \begin{cases} 1 & \text{if } u = wvw \text{ or } v = wuw \text{ for some } w \in \mathbb{Q}\langle a, b \rangle \\ 0, & \text{otherwise} \end{cases}\end{aligned}$$

and extend by linearity. It is easy to check that these satisfy the requirements of inner products.

**Example 2.8.** By considering the trivial inner product of the depth 3 components of  $\sigma_{11}$  and  $\{\sigma_3, \{\sigma_3, \sigma_5\}\}$ , and demanding that these be orthogonal, we find the following canonical decomposition of  $\sigma_{11}$ :

$$\begin{aligned}\sigma_{11} &= \psi_{11} - \frac{1}{264}\{\psi_{-1}, \{\psi_{-1}, \psi_{13}\}\} - \frac{241}{2112}\{\psi_9, \{\psi_3, \psi_{-1}\}\} \\ &+ \frac{479}{2112}\{\psi_7, \{\psi_5, \psi_{-1}\}\} - \frac{2053}{6336}\{\psi_5, \{\psi_7, \psi_{-1}\}\} - \frac{2620903}{9649216}\{\sigma_3, \{\sigma_3, \sigma_5\}\} + \dots\end{aligned}$$

where we have omitted terms of depth 5 (that are uniquely determined), and where  $\psi_{2n+1}$  is given by Definition 2.14.

**Remark 2.9.** One should note that the denominators of coefficients fixed by this method tend to be quite large, with few prime factors. It remains unclear as to whether there is a meaningful reason for this. We suspect it to merely be an artifact of the calculation, as the numbers involved grow quite rapidly.

The first has the advantage of being easy to calculate, with monomials of different weights and depths being orthogonal, while the second is, in some sense, “compatible” with the obvious Lie algebra structure on  $\mathbb{Q}\langle a, b \rangle$ .

**Lemma 2.10** (K.).

$$\langle [w, u], v \rangle_S + \langle u, [w, v] \rangle_S = 0 \text{ for all } u, v, w \in \mathbb{Q}\langle a, b \rangle$$

*Proof.* Follows simply by considering cases. We shall do an example case, to illustrate the method. We have that the LHS is

$$\langle wu, v \rangle - \langle uw, v \rangle + \langle u, wv \rangle - \langle u, vw \rangle$$

For the first term to be non-zero, we must have  $wu = svs$  for some word  $s$ . Then either  $s = wu'$  or  $w = sv'$  where  $u = u'u''$  and  $v = v'v''$ . In the first case, we must have  $u'' = vs$ . Thus

$$\begin{aligned}u &= u'u'' \\ &= u'vs \\ &= u'vwu'\end{aligned}$$

In the second case, we must then have  $u = v''s$ . Thus

$$\begin{aligned}vw &= v'v''sv' \\ &= v'uv'\end{aligned}$$

Hence the fourth term is non-zero and cancels out the first. Similarly, if either of the middle brackets are non-zero, so is the other and they cancel each other out. Thus the sum is constantly 0.  $\square$

**Remark 2.11.** While this "symmetric" inner product  $\langle \cdot, \cdot \rangle_{\mathcal{S}}$  is compatible with the obvious Lie algebra structure on  $\mathbb{Q}\langle a, b \rangle$ , it is *not* compatible with the Ihara bracket. Indeed, it would be particularly interesting to find such an inner product. Evidence coming from the work of Pollack [29] suggests the existence of one, but gives no hints as to how to construct it.

**Remark 2.12.** One should note that, while the trivial inner product seems rather unnatural, it actually has Hodge theoretic origins. It arises from morphism of Lie algebras

$$i : \mathfrak{g} \rightarrow \text{Der}^{\Theta} \mathbb{L}(a, b)$$

where  $\text{Der}^{\Theta}$  denotes the set of derivations  $\delta$  such that  $\delta([a, b]) = 0$ . This morphism, due to the work of Hain [22] and Brown [9], is known to be injective, and creates further ties to the work of Pollack [29]. To be precise,  $i(\sigma_{2n+1}) = \epsilon_{2n+2}^{\vee}$  modulo  $W_{-2n-3}$ , where  $W$  is the geometric weight filtration associated to the mixed Hodge structure of the first order Tate curve  $E_{\frac{\partial}{\partial q}}^{\times}$ .

Here  $\epsilon_{2n}^{\vee} \in \text{Der}^{\Theta} \mathbb{L}(a, b)$  is the derivation defined by

$$\epsilon_{2n}^{\vee}(a) = \text{ad}(a)^{2n}(b) \text{ for } n \geq 1$$

and the fact that it is homogeneous of degree  $2n$  in  $a, b$ . Defining

$$\epsilon_0^{\vee}(a) = b \quad \epsilon_0^{\vee}(b) = 0$$

and denoting by  $\mathfrak{u}^{geom}$  the Lie subalgebra generated by the  $\epsilon_{2n}^{\vee}$ ,  $n \geq 1$ , we obtain the object of study in the work of Pollack. While  $i(\mathfrak{g}) \not\subset \mathfrak{u}^{geom}$ , in low depth, the epsilons give "coordinates" with which to describe the  $\sigma_{2n+1}$ . Furthermore, the relations between elements of  $\mathfrak{u}^{geom}$  give relations between the elements of  $\mathfrak{g}$  modulo higher depths, and create ties with the theory of modular forms. This shall be discussed in greater depth later in this thesis.

Another approach to defining canonical generators involves allowing polar solutions to the double shuffle equations [8]:

$$s^{(1)} = \frac{1}{2x_1} \text{ and } s^{(2)} = \frac{1}{12} \left( \frac{1}{x_1 x_2} + \frac{1}{x_2(x_1 - x_2)} \right)$$

is a solution to the double shuffle equations mod products in depths one and two. By taking the Ihara bracket of  $s$  with various solutions, we can define an "anatomical" decomposition for  $\sigma_{2k-1}$ .

**Definition 2.13.** For any sets of indices  $A, B \subset \{0, \dots, d\}$ , write

$$x_{A,B} = \prod_{a \in A, b \in B} (x_a - x_b)$$

If  $A$  or  $B$  is the empty set, define  $x_{A,B} = 1$ . Define also  $x_0 = 0$

**Definition 2.14.** For every  $n, d \geq 1$ , define  $\psi_{2n+1}^{(d)} \in \mathbb{Q}(x_1, \dots, x_d)$  by

$$\begin{aligned} \psi_{2n+1}^{(d)} = & \frac{1}{2} \sum_{i=1}^d \left( \frac{(x_i - x_{i-1})^{2n}}{x_{\{0, \dots, i-2\}, \{i-1\}} x_{\{i+1, \dots, d\}, \{i\}}} + \frac{x_d^{2n}}{x_{\{1, \dots, i-1\}, \{0\}} x_{\{i, \dots, d-1\}, \{d\}}} \right) \\ & + \frac{1}{2} \sum_{i=1}^{d-1} \left( \frac{(x_1 - x_d)^{2n}}{x_{\{2, \dots, i\}, \{1\}} x_{\{i+1, \dots, d-1, 0\}, \{d\}}} + \frac{x_{d-1}^{2n}}{x_{\{d, 1, \dots, i-1\}, \{0\}} x_{\{i, \dots, d-2\}, \{d-1\}}} \right) \end{aligned}$$

Let  $\psi_{2n+1}$  be the element whose depth  $d$  component is  $\psi_{2n+1}^{(d)}$ .

**Proposition 2.15** (Brown).  $\psi_{2n+1}$  are solutions to the double shuffle equations mod products.

It is possible to write  $\sigma_3, \dots, \sigma_9$  uniquely as Ihara brackets of  $s$  and the  $\psi_{2n+1}$ . Defining  $\psi_{-1} := s$ , we can similarly decompose  $\sigma_{11}$ .

**Example 2.16.**

$$\begin{aligned} \sigma_{11} = & \psi_{11} - \frac{1}{264} \{\psi_{-1}, \{\psi_{-1}, \psi_{13}\}\} - \frac{241}{2112} \{\psi_9, \{\psi_3, \psi_{-1}\}\} \\ & + \frac{479}{2112} \{\psi_7, \{\psi_5, \psi_{-1}\}\} - \frac{2053}{6336} \{\psi_5, \{\psi_7, \psi_{-1}\}\} + \{\text{depth} \geq 5\} \end{aligned}$$

*A priori*  $\sigma_{11}$  is only defined up to multiples of  $\{\sigma_3, \{\sigma_3, \sigma_5\}\}$ . However, by demanding that, in depth three,  $\sigma_{11}$  be written as a sum of brackets  $\{\psi_{a_1}, \{\psi_{a_2}, \psi_{a_3}\}\}$  with at least one of  $\{a_1, a_2, a_3\}$  equal to  $-1$ , we obtain a canonical generator in weight 11, modulo high depths.

However this approach has only been examined on a case by case basis, with no general theory. Polar solutions still make an appearance in the existence of canonical generators: Brown [9] defines canonical  $\sigma_{2k+1}$  up to depth 3 using polar solutions. To be precise, he defines them as follows.

**Definition 2.17.** For all  $n \geq -1$ , define rational functions by

$$\begin{aligned} \xi_{2n+1}^{(1)} &= x_1^{2n} \\ \xi_{2n+1}^{(2)} &= \{s^{(1)}, x_1^{2n}\} \\ \xi_{2n+1}^{(3)} &= \{s^{(2)}, x_1^{2n}\} + \frac{1}{2} \{s^{(1)}, \{s^{(1)}, x_1^{2n}\}\} \end{aligned}$$

Note that we can extend  $\xi_{2n+1}$  to all depths by  $\xi_{2n+1} = \exp(\text{ad}(s))x_1^{2n}$  if we extend  $s$  to a solution in all depths.

**Definition 2.18.** Define canonical generators up to depth three by

$$\sigma_{2n+1}^c = \xi_{2n+1} + \sum_{a+b=n} \binom{2n}{2a} \frac{B_{2a}B_{2b}}{12B_{2n}} \{\xi_{2a+1}, \{\xi_{2b+1}, \xi_{-1}\}\}$$

where  $B_{2n}$  is the  $2n^{\text{th}}$  Bernoulli number.

In [9], Brown shows the following

**Proposition 2.19** (Brown).  $\sigma_{2n+1}^c$  solve the double shuffle equations mod products up to depth three, and have no poles, thus defining genuine elements of  $\mathfrak{dmt}_0$ .

These generators give interesting ties to  $\mathfrak{sl}_2$  and period polynomials, that also arise in the work of Pollack [29]. Specifically, the coefficients appearing in the expression are proportional to those of the odd part of the period polynomial for the Eisenstein series of weight  $2n$ , which is proportional to:

$$\sum_{a+b=n, a,b \geq 1} \binom{2n}{2a} B_{2a}B_{2b} X^{2a-1} Y^{2b-1} \in \mathbb{Q}[X, Y]$$

One thing of note would be if an inner product produced the same canonical generators as one of the other methods. We have checked that the “anatomical” decomposition, and the trivial inner product give distinct generators, but it has yet to be checked in other cases.

### 2.3 The duality phenomenon

One phenomenon amongst elements of  $\mathfrak{d}\mathfrak{mr}_0$  is that of *duality*.

**Definition 2.20.** Define the following linear maps on  $\mathbb{Q}\langle a, b \rangle$

- $R(u_1 u_2 \dots u_n) := u_n u_{n-1} \dots u_1$
- $S$  is the homomorphism defined by  $Sa := b$  and  $Sb := a$
- $D := RS = SR$

We say  $\sigma$  satisfies *duality* if  $\sigma = D\sigma$ .

We have  $\zeta(w) = \zeta(Dw)$ , which we expect: this is just swapping the roles of 0 and 1 in  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . What is unexpected is that we seem to have  $\sigma = D\sigma$  for all  $\sigma \in \mathfrak{d}\mathfrak{mr}_0$ . It is not currently known if duality is a consequence of the double shuffle relations, but numerical evidence seems to suggest it must be.

**Remark 2.21.** The map  $R$  defined here is, up to a sign, the antipode map in the shuffle Hopf algebra  $\mathbb{Q}\langle a, b \rangle$ .

We do, however, know that duality plays nicely with many of the structures on  $\mathfrak{d}\mathfrak{mr}_0$ :  $D$  passes through the motivic coaction [6] and duality is preserved by the Ihara bracket. While this latter fact follows from Brown's proof that the Ihara action is motivic [7], and Racinet's thesis [30], we present a direct proof of it.

**Lemma 2.22** (K.). *If  $\phi(a, b) \in \mathbb{Q}\langle a, b \rangle$  satisfies the shuffle equations mod products, then  $D\phi(a, b) = -\phi(-b, -a)$*

*Proof.* If  $\phi(a, b)$  satisfies the shuffle equations mod products, we must have

$$\phi(a, b) + R\phi(-a, -b) = 0$$

Applying  $D$  to this proves our result. □

**Theorem 2.23** (K.). *Duality is preserved in  $\mathfrak{d}\mathfrak{mr}_0$  by the Ihara bracket.*

*Proof.* The Ihara bracket of two elements is defined by

$$\{\phi_1, \phi_2\} := d_{\phi_2} \phi_1 - d_{\phi_1} \phi_2 - [\phi_1, \phi_2]$$

where  $d_\phi$  is the derivation defined on generators by

$$d_\phi(a) = 0$$

$$d_\phi(b) = [b, \phi]$$

Now suppose  $\phi_1, \phi_2 \in \mathfrak{d}\mathfrak{mr}_0$  satisfy duality, and consider  $\{\phi_1, \phi_2\}(-b, -a)$  We have the following:

$$[\phi_1, \phi_2](-b, -a) = [\phi_1, \phi_2]$$

Next define a derivation  $d'_\phi$  by

$$d'_\phi(a) = [a, \phi]$$

$$d'_\phi(b) = 0$$

We can easily show by induction on the length of  $\phi$  that  $d_\phi(X)(-b, -a) = d'_\phi(X(-b, -a))$  and hence

$$d_{\phi_i}(\phi_j)(-b, -a) = -d'_{\phi_i}(\phi_j) \text{ for } (i, j) \in \{(1, 2); (2, 1)\}$$

One can then check easily that  $d'_{\phi}(X) = d_{\phi}(X) - [X, \phi]$ , by induction, and hence

$$(d_{\phi_1}(\phi_1) - d_{\phi_2}(\phi_1))(-b, -a) = -d_{\phi_1}(\phi_1) + d_{\phi_2}(\phi_1) + 2[\phi_1, \phi_2]$$

and so  $D\{\phi_1, \phi_2\} = -\{\phi_1, \phi_2\}(-b, -a) = \{\phi_1, \phi_2\}$ .  $\square$

We can also make steps towards a proof that duality holds for all elements of  $\mathfrak{dmr}_0$ . To be precise, we can show that it holds for elements of  $\mathfrak{g}^m$ , with minor assumptions. It, in fact, follows from the definition as  $\mathfrak{g}^m$  encodes all motivic relations; in particular, it encodes all relations arising from linearity and functoriality of integration. However, we once again provide a more direct proof, as the proof, with some further assumptions, extend to  $\mathfrak{dmr}_0$ . We first note that  $D$  preserves solutions to the shuffle equations.

**Lemma 2.24** (K.). *If  $\phi(a, b) \in \mathbb{Q}\langle a, b \rangle$  satisfies the shuffle equations mod products, then so does  $D\phi$ .*

*Proof.* One can easily check that

$$(R \otimes R) \circ \Delta = \Delta \circ R$$

and

$$(S \otimes S) \circ \Delta = \Delta \circ S$$

Thus

$$(D \otimes D) \circ \Delta = \Delta \circ D$$

proving our result.  $\square$

We can now show the following.

**Proposition 2.25** (K.). *Suppose  $\sigma_3, \dots, \sigma_{2k-1}$  satisfy duality. Suppose also that  $D\sigma_{2k+1} \in \mathfrak{g}$ . Then  $\sigma_{2k+1}$  satisfies duality.*

*Proof.* By our assumption,  $D\sigma_{2k+1}$  must be in the span of  $\sigma_{2k+1}$  and brackets of lower weight generators. Thus, there exists  $\alpha \in \mathbb{Q}$  such that  $\sigma_{2k+1} - \alpha D\sigma_{2k+1}$  is a linear combination of brackets of lower weight generators. By the previous theorem,  $\sigma_{2k+1} - \alpha D\sigma_{2k+1}$  must satisfy duality and thus

$$(\alpha + 1)\sigma_{2k+1} = (\alpha + 1)D\sigma_{2k+1}$$

Then, as  $\mathfrak{g} \subset \mathfrak{dmr}_0$ , we obtain from the stuffle equation and translation invariance of  $\sigma_{2k+1}$ , evaluated at  $x_1 = 1, x_i = 0 \ i = 2, 3, \dots, 2k$ , that

$$\begin{aligned} (\sigma_{2k+1}|ab^{2k}) &= -(\sigma_{2k+1}|bab^{2k-1}) - (\sigma_{2k+1}|b^2ab^{2k-2}) - \dots - (\sigma_{2k+1}|b^{2k}a) \\ &= \sum_{i=1}^{2k-1} (\sigma_{2k+1}|b^i a^2 b^{2k-1-i}) \\ &\vdots \\ &= (-1)^{2k} (\sigma_{2k+1}|b^{2k}a) = (\sigma_{2k+1}|a^{2k}b) \end{aligned}$$

and so

$$(D\sigma_{2k+1}|a^{2k}b) = (\sigma_{2k+1}|ab^{2k}) = (\sigma_{2k+1}|a^{2k}b)$$

Thus, we must have  $\alpha = 1$  and so  $\sigma_{2k+1} = D\sigma_{2k+1}$   $\square$

One could alter the assumptions made about  $D\sigma_{2k+1}$ , however, it is not clear that the altered assumptions would be weaker. For example, if we simply take  $D\sigma_{2k+1} \in \mathfrak{dmr}_0$  [32] we have to make certain assumptions about the nature of  $\mathfrak{dmr}_0$  in order to follow the same proof method. Note also that we cannot replace  $\sigma_{2k+1}$  by an arbitrary element, as we rely on having non-zero depth one components, and in this,  $\sigma$ -elements are near unique in  $\mathfrak{dmr}_0$ .

We also get an interesting interplay between duality and the proposed symmetric inner product. We first note the following trivial fact.

**Lemma 2.26** (K.).

$$\langle Du, Dv \rangle_S = \langle u, v \rangle_S$$

**Definition 2.27.** Given an inner product  $\langle \cdot, \cdot \rangle_S$ , define

$$\langle u, v \rangle_m = \begin{cases} \langle u, v \rangle_S & \text{if } u, v \text{ are both of odd depth} \\ -\langle u, v \rangle_S & \text{if } u, v \text{ are both of even depth} \\ 0 & \text{otherwise} \end{cases}$$

**Definition 2.28.** Define  $\mathbb{Q}^o\langle a, b \rangle$  to be the subspace of  $\mathbb{Q}\langle a, b \rangle$  consisting of polynomials with monomials only of odd weight.

Let  $\mathbb{Q}^D\langle a, b \rangle$  be the subspace of  $\mathbb{Q}^o\langle a, b \rangle$  consisting of polynomials equal to their duals.

Let  $\mathbb{Q}^O\langle a, b \rangle$  be the subspace of  $\mathbb{Q}^o\langle a, b \rangle$  consisting of polynomials with monomials only of odd depth. Note that we have a surjection  $\pi : \mathbb{Q}^D\langle a, b \rangle \rightarrow \mathbb{Q}^O\langle a, b \rangle$ .

**Lemma 2.29** (K.).  $\langle \sigma, \rho \rangle_m = 0$  for all  $\sigma, \rho \in \mathbb{Q}^D\langle a, b \rangle$ .

*Proof.* We have

$$\langle \sigma, \rho \rangle_m = \langle \sigma_{\text{odd}}, \rho_{\text{odd}} \rangle_S - \langle \sigma_{\text{even}}, \rho_{\text{even}} \rangle_S$$

As duality swaps the parity of depth of elements of  $\mathbb{Q}^o\langle a, b \rangle$ , we get that

$$\begin{aligned} \langle \sigma, \rho \rangle_m &= \langle \sigma_{\text{odd}}, \rho_{\text{odd}} \rangle_S - \langle D\sigma_{\text{odd}}, D\rho_{\text{odd}} \rangle_S \\ &= \langle \sigma_{\text{odd}}, \rho_{\text{odd}} \rangle_S - \langle \sigma_{\text{odd}}, \rho_{\text{odd}} \rangle_S = 0 \end{aligned}$$

□

**Lemma 2.30** (K.). If  $\langle \sigma, \rho \rangle_m = 0$  for all  $\rho \in \mathbb{Q}^D\langle a, b \rangle$ , then  $\sigma \in \mathbb{Q}^D\langle a, b \rangle$ .

*Proof.*

$$\begin{aligned} \langle \sigma, \rho \rangle_m = 0 \quad \forall \rho \in \mathbb{Q}^D\langle a, b \rangle &\Rightarrow \langle \sigma_{\text{odd}}, \rho_{\text{odd}} \rangle_S = \langle \sigma_{\text{even}}, \rho_{\text{even}} \rangle_S \quad \forall \rho \in \mathbb{Q}^D\langle a, b \rangle \\ &\Rightarrow \langle \sigma_{\text{odd}}, \rho_{\text{odd}} \rangle_S = \langle D\sigma_{\text{even}}, \rho_{\text{odd}} \rangle_S \quad \forall \rho \in \mathbb{Q}^D\langle a, b \rangle \\ &\Rightarrow \langle \sigma_{\text{odd}} - D\sigma_{\text{even}}, \rho_{\text{odd}} \rangle_S = 0 \quad \forall \rho_{\text{odd}} \in \mathbb{Q}^O\langle a, b \rangle \end{aligned}$$

Then, as  $\langle \cdot, \cdot \rangle_S$  is a nondegenerate inner product on  $\mathbb{Q}^O\langle a, b \rangle$ , we must have

$$\sigma_{\text{odd}} = D\sigma_{\text{even}}$$

which implies

$$\sigma = D\sigma$$

as  $D^2 = D$ .

□

**Theorem 2.31** (K.).

$$\mathbb{Q}^D\langle a, b \rangle = \bigcap_{\rho \in \mathbb{Q}^D\langle a, b \rangle} \ker \langle \cdot, \rho \rangle_S$$

So the symmetric inner product in some sense "cuts out" polynomials satisfying duality. Unfortunately, this fact is computationally ineffective, but still interesting.

## 2.4 Linearised double shuffle equations

While the double shuffle equations are homogeneous for weight, they are not homogeneous for depth. Rather, the shuffle equations are, but the stuffle equations are not. As such, we can further simplify our equations by taking the associated graded of  $\mathfrak{d}\mathfrak{mr}_0$  with respect to the depth filtration, to obtain  $\mathfrak{d}\mathfrak{g}$ . This is no longer a free Lie algebra, as we now obtain relations among  $\bar{\sigma}_{2i+1}$ , the images of  $\sigma_{2n+1}$ , identical to those of Pollack [29]. However, the equations describing elements of  $\mathfrak{d}\mathfrak{g}$  become much simpler. Indeed, we have  $\mathfrak{d}\mathfrak{g} \subset \mathfrak{ls}$ , the space of solutions to the *linearised double shuffle equations* [7].

**Definition 2.32.** We say  $\sigma \in k\langle a, b \rangle$  satisfies the linearised double shuffle equations if the following conditions hold:

$$\begin{aligned}\Delta\sigma &= \sigma \otimes 1 + 1 \otimes \sigma \\ \Delta_*^{\mathfrak{ls}} \pi_Y \sigma &= \pi_Y \sigma \otimes 1 + 1 \otimes \pi_Y \sigma \\ (\sigma|a) &= (\sigma|b) = (\sigma|ab) = 0\end{aligned}$$

where  $\Delta_*^{\mathfrak{ls}} : k\langle Y \rangle \rightarrow k\langle Y \rangle \otimes k\langle Y \rangle$  is defined on generators by

$$\Delta_*^{\mathfrak{ls}}(y_i) := y_i \otimes 1 + 1 \otimes y_i$$

We denote the space of solutions to the linearised double shuffle equations by  $\mathfrak{ls}$ .

**Proposition 2.33** (Brown).  *$\mathfrak{ls}$  equipped with the Ihara bracket forms a Lie algebra.*

We can once again translate this into the language of commutative variables.

**Definition 2.34.** We say  $f \in k[x_1, \dots, x_n]$  solves the linearised double shuffle equations if

$$\begin{aligned}f^\#(\mathbf{x}_1 \dots \mathbf{x}_i \sqcup \mathbf{x}_{i+1} \dots \mathbf{x}_n) &= 0 \\ f(\mathbf{x}_1 \dots \mathbf{x}_i \sqcup \mathbf{x}_{i+1} \dots \mathbf{x}_n) &= 0\end{aligned}$$

**Remark 2.35.** Note that we have Sh in both the linearised shuffle and linearised stuffle equations. The primary distinction between Sh and  $\star$  is the lower depth terms, which disappear in the linearisation.

**Remark 2.36.** Note that we can now assume  $\sigma \in \mathfrak{ls}$  to be homogeneous in weight *and* depth, as our equations are now homogeneous in both.

While it is not immediately obvious that moving to the linearised double shuffle equations achieves anything of note, one can translate several important conjectures into conjectures about the nature of  $\mathfrak{d}\mathfrak{g}$  and  $\mathfrak{ls}$ . For example, Brown [7] defines an explicit injective linear map

$$\mathbf{e} : S_{2n} \rightarrow \mathfrak{ls}$$

where  $S_{2n} \subset \mathbb{Q}[X, Y]$  is the vector space of even period polynomials.

**Definition 2.37.** Define  $S_{2n} \subset \mathbb{Q}[X, Y]$  to be the vector space of antisymmetric homogeneous polynomials  $P(X, Y)$  of degree  $2n - 2$  satisfying

$$\begin{aligned}P(X, 0) &= 0 \\ P(\pm X, \pm Y) &= P(X, Y) \\ P(X, Y) + P(X - Y, X) + P(-Y, X - Y) &= 0\end{aligned}$$

This map provides a reformulation of the (depth graded) Broadhurst-Kreimer conjecture on the dimensions of  $\mathfrak{d}\mathfrak{g}$ :

**Conjecture 2.38.** The image of  $\mathbf{e}$  lies in  $\mathfrak{dg}$  and

$$\begin{aligned} H_1(\mathfrak{dg}; \mathbb{Q}) &\cong \bigoplus_{i \geq 1} \bar{\sigma}_{2i+1} \mathbb{Q} \oplus \bigoplus_{n \geq 1} (e)(S_{2n}) \\ H_2(\mathfrak{dg}; \mathbb{Q}) &\cong \bigoplus_{n \geq 1} S_{2n} \\ H_i(\mathfrak{dg}; \mathbb{Q}) &= 0 \text{ for all } i \geq 3 \end{aligned}$$

This can be made into a much stronger conjecture about the homology of  $\mathfrak{ls}$ .

**Conjecture 2.39.** Denoting by  $\mathfrak{ls}_1$  the depth 1 component of  $\mathfrak{ls}$ , and by  $S := \bigoplus_{n \geq 1} S_{2n}$ , it is conjectured that the following holds:

$$\begin{aligned} H_1(\mathfrak{ls}; \mathbb{Q}) &\cong \mathfrak{ls}_1 \oplus \mathbf{e}(S) \\ H_2(\mathfrak{ls}; \mathbb{Q}) &\cong S \\ H_i(\mathfrak{ls}; \mathbb{Q}) &= 0 \text{ for all } i \geq 3 \end{aligned}$$

Conjecturally, these are equivalent: it is believed that  $\mathfrak{dg} \cong \mathfrak{ls}$ . Both would imply the following conjecture on the dimensions of  $\mathfrak{dg}$ .

**Conjecture 2.40.** Denoting by  $\mathcal{D}$  the depth filtration, we have

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

where

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

Here  $\mathbb{E}(s)$  and  $\mathbb{O}(s)$  are the generating series of the dimensions of spaces of even and odd single zeta values respectively.  $\mathbb{S}(s)$  has an interpretation as the generating series for the graded dimensions of the space of cusp forms for the full modular group  $PSL_2(\mathbb{Z})$ .

This conjecture makes the connection with period polynomials and modular forms slightly more explicit. However, it is not clear precisely why the connection exists.

Still, the study of solutions to the linearised double shuffle equations gives powerful machinery, such as the depth-parity theorem [7].

**Proposition 2.41.** Suppose  $\sigma \in \mathfrak{ls}$  is of weight  $N$  and depth  $d$ . Then, if  $N$  and  $d$  are of opposite parity,  $\sigma = 0$ . That is, there are no non-trivial solutions to the linearised double shuffle equations with weight and depth of opposite parity.

This in turn gives use a method for tackling so called “totally odd” multiple zeta values [7],[14]. Multiple lower bounds for the dimensions of the space of totally odd multiple zeta values have been given. However, as the notation involved is quite particular, we mention this only as an aside.

Another useful corollary of the depth parity theorem is the following.

**Corollary 2.42.** For a solution to the double shuffle equations mod products  $\phi \in \mathfrak{dmr}_0$ , of weight  $N$ , the depth  $d + 1 \not\equiv N \pmod{2}$  components are uniquely determined by the lower depths. In particular,  $\sigma_{2n+1}$  is uniquely determined in depths 1 and 2.

*Proof.* Suppose  $\phi_1$  and  $\phi_2$  are of weight  $N$  and agree up to depth  $d \equiv N \pmod{2}$ . Then the depth  $d + 1$  component of  $\phi_1 - \phi_2$  is a solution to the linearised double shuffle equations and hence, by the depth parity theorem, is 0. Thus  $\phi_1$  and  $\phi_2$  agree up to depth  $d + 1$  and the depth  $d + 1$  component is uniquely determined.  $\square$

**Remark 2.43.** It would be interesting if this corollary could be “dualised”: if we assume that the duality operator preserves  $\mathfrak{d}\mathbf{mr}_0$ , then we must have that the depth  $d-1 \not\equiv N \pmod{2}$  component of a weight  $N$  element of  $\mathfrak{d}\mathbf{mr}_0$  is uniquely determined by the higher depths, suggesting that a top down approach may be a viable option in solving the double shuffle equations mod products.

## 2.5 Relations and obstructions from period polynomials

One of the challenges in defining canonical  $\sigma$  elements, and in working with  $\mathfrak{ls}$  is the existence of relations between  $\sigma$  elements in low depth, such as Ihara’s relation

$$3\{\sigma_5, \sigma_7\} = \{\sigma_3, \sigma_9\} \text{ modulo depths } \geq 4$$

However, we can explicitly describe all quadratic relations, as they all arise from period polynomials [21], [29].

Our map  $\rho : \mathbb{Q}\langle a, b \rangle \rightarrow \bigoplus_{n=1}^{\infty} \mathbb{Q}[y_0, \dots, y_n]$  descends to a map

$$\bar{\rho} : \mathfrak{ls} \rightarrow \bigoplus_{n=1}^{\infty} \mathbb{Q}[y_0, \dots, y_n] \rightarrow \bigoplus_{n=1}^{\infty} \mathbb{Q}[x_1, \dots, x_n]$$

The Ihara bracket gives a map

$$\{\cdot, \cdot\} : \mathfrak{ls}_1 \wedge \mathfrak{ls}_1 \rightarrow \mathfrak{ls}_2$$

which on application of  $\bar{\rho}$  gives a map

$$D_1 \wedge D_1 \rightarrow D_2$$

where  $D_i$  is the  $\mathbb{Q}$ -vector space of even polynomials in  $i$  variables. We find that  $D_1 \wedge D_1$  is isomorphic to the space of antisymmetric even polynomials  $p(x_1, x_2)$ . The image of  $p(x_1, x_2)$  under the induced map is

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

Recalling Definition 2.37, we conclude that the kernel of this map is isomorphic to  $S$ . In fact, one can show relatively easily that the following sequence is exact:

$$0 \rightarrow S \rightarrow D_1 \wedge D_1 \rightarrow D_2 \rightarrow 0$$

**Example 2.44.** The smallest non-trivial period polynomial, arising from the cusp form of weight 12, is given by  $s_1 2 = X^8 Y^2 - 3X^6 Y^4 + 3X^4 Y^6 - X^2 Y^8$ . From the short exact sequence, and the isomorphism  $\bar{\rho}$ , we can immediately see Ihara’s relation:

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

Using the map  $\mathfrak{ls} \rightarrow \text{Der}^{\Theta} \mathbb{L}(a, b)$  that sends  $\bar{\sigma}_{2n+1}$  to  $\epsilon_{2n+2}^{\vee}$ , we can apply Pollack’s work to describe all such quadratic relations and their connection to modular forms.

**Definition 2.45.** For  $f$  a cusp form of weight  $n$ , define the period polynomial of  $f$  to be

$$r_f(X, Y) = \sum a_f(k) X^{n-2-k} Y^k = \int_0^{i\infty} f(\tau) (X - \tau Y)^{n-2} d\tau$$

In [34], Zagier extends this definition to all modular forms. Denote by

$$r_f^+ = \frac{1}{2}(r_f(X, Y) + r_f(X, -Y))$$

the even degree part of  $r_f$ . This is an element of  $S$ . In his thesis, Pollack shows the following, as a special case of his main theorem.

**Theorem 2.46.** *For  $n$  a fixed positive even integer*

$$\sum_{p+q=n+2} \beta(p, q)[\epsilon_p^\vee, \epsilon_q^\vee] = 0$$

*if and only if there exists a modular form  $f$  of weight  $n$  such that*

$$r_f^+(X, Y) = \sum_{p+q=n+2} \beta(p, q)(X^{p-2}Y^{q-2} - X^{q-2}Y^{p-2})$$

This gives us a way of generating relations, in fact all quadratic relations, among the  $\bar{\sigma}_{2n+1}$ .

**Example 2.47.** The relation

$$2\{\bar{\sigma}_3, \bar{\sigma}_{13}\} - 7\{\bar{\sigma}_5, \bar{\sigma}_{11}\} + 11\{\bar{\sigma}_7, \bar{\sigma}_9\} = 0$$

arises from the cusp form of weight 16, with even period polynomial

$$2(X^2Y^{12} - X^{12}Y^2) - 7(X^4Y^{10} - X^{10}Y^4) + 11(X^6Y^8 - X^8Y^6)$$

Modular forms and period polynomials also play a role in defining *exceptional generators*. The map

$$\mathbf{e} : \mathbf{S} \rightarrow \mathbf{ls}$$

defines elements  $\mathbf{e}_f \in \mathbf{ls}$  that in some sense describe the failure of relations in  $\mathbf{ls}$  to hold in  $\mathfrak{dmr}_0$ . For example

$$3\{\sigma_5, \sigma_7\} - \{\sigma_3, \sigma_9\} \in \mathbb{Q}\mathbf{e}_f$$

for  $f$  the cusp form of weight 12. Thus, these exceptional elements become vital in computation of the dimension of solution spaces to the double shuffle equations. In fact, we have that the Conjecture 2.38 is equivalent to showing that  $\mathbf{e}(S) \subset \mathfrak{dg}$ , which was verified by Brown up to weight 20, and that the Lie subalgebra of  $\mathfrak{dg}$  generated by the elements  $\text{ad}^{2n}(a)(b)$  and  $\mathbf{e}_f$  has the homology described in Conjecture 2.38.

### 3 The block filtration and block graded multiple zeta values

#### 3.1 The block filtration

In addition to the weight and depth filtrations, we will define a ‘block filtration’ on (motivic) multiple zeta values, arising from the work of Charlton [10] in his thesis. In his thesis, Charlton defines the block decomposition of a word in two letters  $\{x, y\}$  as follows.

Begin by defining a word in  $\{x, y\}$  to be *alternating* if it is non empty and has no subsequences of the form  $xx$  or  $yy$ . There are exactly two alternating words of any given length: one beginning with  $x$  and one beginning with  $y$ . Charlton shows that every non-empty word  $w \in \{x, y\}^\times$  can be written uniquely as a minimal concatenation of alternating words. In particular, he defines the block decomposition  $w = w_1 w_2 \dots w_k$  as the unique factorisation into alternating words such that the last letter of  $w_i$  equals the first letter of  $w_{i+1}$ .

We can use this to define a degree function on words in two letters.

**Definition 3.1.** Let  $w \in \{x, y\}^\times$  be a word of length  $n$ , given by  $w = a_1 \dots a_n$ . Define its block degree  $\deg_{\mathcal{B}}(w)$  to be one less than the number of alternating words in its block decomposition. Equivalently, define

$$\deg_{\mathcal{B}}(w) := \#\{i : 1 \leq i < n \text{ such that } a_i = a_{i+1}\}$$

**Remark 3.2.** Note that, unlike depth, the block degree of a word is preserved by the duality anti-homomorphism, mapping  $e_0 \leftrightarrow e_1$ , induced by the automorphism  $z \mapsto 1 - z$  of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ .

We can then define an increasing filtration on  $\mathbb{Q}\langle e_0, e_1 \rangle$  by

$$\mathcal{B}_n \mathbb{Q}\langle e_0, e_1 \rangle := \langle w : \deg_{\mathcal{B}}(w) \leq n \rangle_{\mathbb{Q}}$$

which, following the suggestion of Brown [4], when restricted to a filtration on  $e_1 \mathbb{Q}\langle e_0, e_1 \rangle e_0$  induces a filtration on motivic multiple zeta values

$$\mathcal{B}_n \mathcal{H} := \langle \zeta^{\mathbf{m}}(w) : w = e_1 u e_0, \deg_{\mathcal{B}}(w) \leq n \rangle_{\mathbb{Q}}$$

Brown goes on to show the following.

**Proposition 3.3** (Brown). *Let  $G_{\mathcal{MT}(\mathbb{Z})}^{\text{dR}}$  denote the de Rham motivic Galois group of the category  $\mathcal{MT}(\mathbb{Z})$ , and let  $U_{\mathcal{MT}(\mathbb{Z})}^{\text{dR}}$  denote its unipotent radical. Then  $\mathcal{B}_n$  is stable under the action of  $G_{\mathcal{MT}(\mathbb{Z})}^{\text{dR}}$ , and  $U_{\mathcal{MT}(\mathbb{Z})}^{\text{dR}}$  acts trivially on  $\text{gr}^{\mathcal{B}} \mathcal{H}$ . Equivalently*

$$\Delta^r(\mathcal{B}_n \mathcal{H}) \subset \mathcal{O}(U_{\mathcal{MT}(\mathbb{Z})}^{\text{dR}}) \otimes \mathcal{B}_{n-1} \mathcal{H}$$

where  $\Delta^r(x) := \Delta(x) - x \otimes 1 - 1 \otimes x$  is the reduced coproduct.

**Corollary 3.4** (Brown). *The block filtration induces the level filtration on the subspace spanned by the Hoffman motivic multiple zeta values  $\zeta^{\mathbf{m}}(n_1, \dots, n_r)$ , with  $n_i \in \{2, 3\}$ , where the level is the number of indices equal to 3.*

*Proof.* The word corresponding to  $(n_1, \dots, n_r)$ , with  $n_i \in \{2, 3\}$  of level  $m$  has exactly  $m$  occurrences of the subsequence  $e_0 e_0$  and none of  $e_1 e_1$ . Therefore, its block degree is exactly  $m + 1$ .  $\square$

As a corollary to this, and Brown’s proof that the Hoffman motivic multiple zeta values form a basis of  $\mathcal{H}$ , we obtain

**Corollary 3.5** (Brown). *Every element in  $\mathcal{B}_n\mathcal{H}$  of weight  $N$  can be written uniquely as a  $\mathbb{Q}$ -linear combination of motivic Hoffman elements of weight  $N$  and level at most  $n$ . Additionally*

$$\sum_{m, n \geq 0} \dim \operatorname{gr}_m^{\mathcal{B}} \mathcal{H}_n s^m t^n = \frac{1}{1 - t^2 - st^3}$$

where  $\mathcal{H}_n$  denotes the weight  $n$  piece of  $\mathcal{H}$ .

However, trying to naively extend this filtration by

$$\mathcal{B}_n\mathcal{H} = \langle \zeta^{\mathfrak{m}}(w) : \deg_{\mathcal{B}}(w) \leq n \rangle_{\mathbb{Q}}$$

we find that the associated graded  $\operatorname{gr}^{\mathcal{B}}\mathcal{H}$  becomes nearly trivial. If we define our filtration as follows, we obtain a much more interesting structure

**Definition 3.6.** We define the block filtration of  $\mathbb{Q}\langle e_0, e_1 \rangle$  by

$$\mathcal{B}_n\mathbb{Q}\langle e_0, e_1 \rangle := \langle w : \deg_{\mathcal{B}}(e_0 w e_1) \leq n \rangle_{\mathbb{Q}}$$

This induces the block filtration of motivic multiple zeta values

$$\mathcal{B}_n\mathcal{H} := \langle \zeta^{\mathfrak{m}}(w) : \deg_{\mathcal{B}}(0w1) \leq n \rangle_{\mathbb{Q}}$$

This filtration agrees with our earlier definition if we restrict to  $w \in e_1\mathbb{Q}\langle e_0, e_1 \rangle e_0$ , but the associated graded remains interesting.

**Proposition 3.7.**

$$\Delta^r \mathcal{B}_n\mathcal{H} \subset \sum_{k=1}^{n-1} \mathcal{B}_k\mathcal{H} \otimes \mathcal{B}_{n-k}\mathcal{H}$$

*Proof.* We will in fact show a stronger statement, that  $\Delta$  is graded for block degree at the level of words. Let  $\mathcal{I} := \langle \mathfrak{I}^{\mathfrak{f}}(0; w; 1) : w \in \{0, 1\}^{\times} \rangle_{\mathbb{Q}}$  be the vector space spanned by formal symbols, with natural projection

$$\begin{aligned} \mathcal{I} &\rightarrow \mathcal{H} \\ \mathfrak{I}^{\mathfrak{f}}(0; w; 1) &\mapsto \mathfrak{I}^{\mathfrak{m}}(0; w; 1) \end{aligned}$$

and, similarly, a natural projection  $\mathcal{I} \rightarrow \mathcal{A}$ .

Recall that the coaction is given by the formula

$$\begin{aligned} \Delta I^{\mathfrak{m}}(a_0; a_1, \dots, a_n; a_{n+1}) &:= \\ \sum_{0=i_0 < i_1 < \dots < i_k < i_{k+1}=n+1} \prod_{p=0}^k I^{\mathfrak{a}}(a_{i_p}; a_{i_p+1}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) &\otimes I^{\mathfrak{m}}(a_0; a_{i_1}, \dots, a_{i_k}; a_{n+1}) \end{aligned}$$

where  $0 \leq k \leq n$ , and the infinitesimal coactions

$$\begin{aligned} D_{2r+1} : \mathcal{H}_N &\rightarrow \mathcal{L}_{2r+1} \otimes \mathcal{H}_{N-2r-1} \\ I^{\mathfrak{m}}(a_0; a_1, \dots, a_N; a_{N+1}) &\mapsto \\ \sum_{p=0}^{N-2r-1} I^{\mathfrak{a}}(a_p; a_{p+1}, \dots, a_{p+2r+1}; a_{p+2r+2}) &\otimes I^{\mathfrak{m}}(a_0; a_1, \dots, a_p, a_{p+2r+2}, \dots, a_N; a_{N+1}) \end{aligned}$$

where  $I^{\mathfrak{a}}$  is taken to be its projection into  $\mathcal{L} := \mathcal{A}_{>0}/\mathcal{A}_{>0}\mathcal{A}_{>0}$ . Note that these lift to coactions  $\mathcal{I} \rightarrow \mathcal{I} \otimes \mathcal{I}$ , by calculating these purely symbolically.

Define  $\mathcal{I}_n := \langle \mathbb{I}^\dagger(0; w; 1) : \deg_{\mathcal{B}}(0w1) = n \rangle_{\mathbb{Q}}$ . It is sufficient to show that  $\Delta \mathcal{I}_n \subset \sum_{i=0}^n \mathcal{I}_i \otimes \mathcal{I}_{n-i}$ , as the result follows upon composition with the necessary projections. In fact, it suffices to show that

$$D_{2r+1} \mathcal{I}_n \subset \sum_{i=0}^n \mathcal{I}_i \otimes \mathcal{I}_{n-i}$$

Now, consider  $\mathbb{I}^\dagger(0; w; 1)$ ,  $w$  a word in  $\{0, 1\}$  such that  $\deg_{\mathcal{B}}(0w1) = n$ . Then we can decompose  $0w1 = b_1 b_2 \dots b_{n+1}$  into alternating blocks, and consider the action of  $D_{2n+1}$  on  $\mathbb{I}^\dagger(b_1 \dots b_{n+1})$ . All terms in  $D_{2n+1} \mathbb{I}^\dagger(b_1 \dots b_{n+1})$  will be of the form

$$\mathbb{I}^\dagger(x; b_i'' b_{i+1} \dots b_{i+j}'; y) \otimes \mathbb{I}^\dagger(b_1 \dots b_{i-1} b_i' x y b_{i+j}'' b_{i+j+1} \dots b_{n+1})$$

for some  $1 \leq i \leq n+1$ , where  $b_i = b_i' x b_i''$ ,  $b_{i+j} = b_{i+j}' y b_{i+j}''$ . For the left hand term to be non-zero, we must have  $x \neq y$ , and so we see

$$\begin{aligned} \deg_{\mathcal{B}}(x b_i'' b_{i+1} \dots b_{i+j}') &= j \\ \deg_{\mathcal{B}}(b_1 \dots b_i' x y b_{i+j}'' \dots b_{n+1}) &= n - j \end{aligned}$$

by counting the blocks. Thus, we get that the total block degree of any term in the coproduct is  $n$ , and the result follows.  $\square$

**Corollary 3.8.** *The block filtration on  $\mathbb{Q}\langle e_0, e_1 \rangle$  induces the coradical filtration on  $\mathcal{H}$ .*

**Corollary 3.9.** *The (linearised) Ihara action  $\circ : \mathbb{Q}\langle e_0, e_1 \rangle \otimes \mathbb{Q}\langle e_0, e_1 \rangle \rightarrow \mathbb{Q}\langle e_0, e_1 \rangle$  is graded for block degree.*

*Proof.* The Ihara action is dual to the motivic coaction. As this proof shows the coaction to be, at the level of words, graded for block degree, the claim follows immediately. One can also show this directly via the recursive formula [8] for the linearised Ihara action.  $\square$

We finish our discussion of the block filtration with a short observation due to Charlton [10], providing an analogue of the depth parity theorem [7].

**Lemma 3.10.** *Let  $w = w_1 \dots w_n$  be a word in  $\{0, 1\}^\times$  of length  $n$ , with  $\deg_{\mathcal{B}}(w) = b$ . Then  $I^m(w) = 0$  if  $b \equiv w + 1 \pmod{2}$ .*

## 3.2 Block-graded multiple zeta values and an encoding of relations

As the block filtration is motivic, and invariant under the duality arising from the symmetry  $z \mapsto 1 - z$  of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ , we can consider the associated graded  $\text{gr}^{\mathcal{B}} \mathcal{A} := \bigoplus_{n=0}^{\infty} \mathcal{B}_n \mathcal{A} / \mathcal{B}_{n-1} \mathcal{A}$ , and to consider block graded motivic multiple zeta values, which we define as follows, following the example of Brown's depth graded multiple zeta values [7]

**Remark 3.11.** In the following it is important to keep in mind that we are indentifying  $e_i \leftrightarrow \frac{dz}{z-i}$ , and, as such, elements of  $\mathfrak{g}^m$  describe relations among iterated integrals, rather than multiple zeta values. As such, our results are 'depth signed' compared to standard notation.

**Definition 3.12.** Define  $\mathcal{B}^n \mathbb{Q}\langle e_0, e_1 \rangle := \langle w : \deg_{\mathcal{B}}(e_0 w e_1) \geq n \rangle_{\mathbb{Q}}$  and define

$$\text{gr}_{\mathcal{B}} \mathfrak{g}^m := \bigoplus_{n=0}^{\infty} \mathcal{B}^n \mathfrak{g}^m / \mathcal{B}^{n+1} \mathfrak{g}^m$$

where we identify  $\mathcal{B}^n \mathfrak{g}^m / \mathcal{B}^{n+1} \mathfrak{g}^m$  with its image in  $\mathcal{B}^n \mathbb{Q}\langle e_0, e_1 \rangle / \mathcal{B}^{n+1} \mathbb{Q}\langle e_0, e_1 \rangle$ , and equip it with the block graded Ihara bracket.

**Definition 3.13.** If  $\deg_{\mathcal{B}}(w) = n$ , define  $\mathbb{I}^{\text{bl}}(0; w; 1)$  to be the image of  $\mathbb{I}^a(0; w; 1)$  in  $\mathcal{B}_n \mathcal{A} / \mathcal{B}_{n-1} \mathcal{A}$ .

**Definition 3.14.** Fix an embedding of  $\{\sigma_3, \sigma_5, \dots\} \hookrightarrow \mathbb{Q}\langle e_0, e_1 \rangle$ . We define the block graded generators  $\{p_{2k+1}\}_{k \geq 1}$  to be the image of the generators  $\{\sigma_{2k+1}\}_{k \geq 1}$  of  $\mathfrak{g}^m$  in  $\mathcal{B}^1\mathbb{Q}\langle e_0, e_1 \rangle / \mathcal{B}^2\mathbb{Q}\langle e_0, e_1 \rangle$ . We define the bigraded Lie algebra  $\mathfrak{bg}$  to be the Lie algebra generated by  $p_{2k+1}$ , equipped with the Ihara bracket.

One of the challenges in studying  $\mathfrak{g}^m$  is that we have an ambiguity in our representation of the generators:  $\sigma_{2k+1}$  is unique only up to addition of another element of weight  $2k+1$ . Its depth one part is canonical, so Brown's depth graded Lie algebra avoids this issue. We find similar success here.

**Proposition 3.15.** *The generators  $p_{2k+1}$  of  $\mathfrak{bg}$  are canonical, i.e. independent of our choice of generators  $\sigma_{2k+1}$  of  $\mathfrak{g}^m$ .*

*Proof.* Let  $\sigma_{2k+1}, \sigma'_{2k+1}$  be two choices of generator for  $\mathfrak{g}^m$  in weight  $2k+1$ . We must have

$$\sigma_{2k+1} - \sigma'_{2k+1} \in \{\mathfrak{g}^m, \{\mathfrak{g}^m, \mathfrak{g}^m\}\}$$

Corollary 3.9 tells us that the Ihara action is compatible with the block filtration, and so

$$\{\mathfrak{g}^m, \{\mathfrak{g}^m, \mathfrak{g}^m\}\} \subset \mathcal{B}^3\mathfrak{g}^m$$

and therefore

$$p_{2k+1} - p'_{2k+1} = 0$$

□

Note that we can still define a concept of depth on  $\mathfrak{bg}$  as before. We define the depth of a word  $w$  to be  $d(w)$ , and induce a decreasing filtration on  $\mathfrak{bg}$  via its embedding  $\mathfrak{bg} \hookrightarrow \mathbb{Q}\langle e_0, e_1 \rangle$ . It is interesting here that depth grading gives canonical generators in depth 1, while block grading gives  $p_{2k+1}$  consisting only of terms of depth  $k, k+1$ .

**Lemma 3.16.**  *$p_{2k+1}$  contains only depth  $k$  and  $k+1$  terms.*

*Proof.* Suppose  $w$  is a word of block degree 1 and weight  $2k+1$ . Then  $e_0 w e_1$  has two blocks, and hence contains exactly one of  $e_0^2$  or  $e_1^2$ . In the first case, the number of  $e_1$  must be exactly half  $2k+1-1$ , i.e.  $k$ . In the second case, the number of  $e_0$  must similarly be  $k$  and hence the number of  $e_1$  is  $k+1$ . □

**Theorem 3.17.**  *$\mathfrak{bg}$  is freely generated by  $\{p_{2k+1}\}_{k \geq 1}$  as a Lie algebra*

*Proof.* We have a bijection between the generators of  $\mathfrak{g}^m$  and of  $\mathfrak{bg}$ , and Corollary 3.9 tells us that the Ihara action is graded for block degree. Thus, we can write an element  $\{p_{2k_1+1}, \{\dots, \{p_{2k_{b-1}+1}, p_{2k_b+1}\}, \dots\}\}$  as the image of  $\{\sigma_{2k_1+1}, \{\dots, \{\sigma_{2k_{b-1}+1}, \sigma_{2k_b+1}\}, \dots\}\}$  in  $\mathcal{B}^b\mathfrak{g}^m / \mathcal{B}^{n+1}\mathfrak{g}^m$ . Hence, we have a relation in  $\mathfrak{bg}$  if and only if the corresponding sum of terms is 0 in  $\text{gr}_{\mathcal{B}}\mathfrak{g}^m$ . Indeed, we have an injective Lie algebra homomorphism  $\mathfrak{bg} \hookrightarrow \text{gr}_{\mathcal{B}}$  induced by the bijection  $\{\sigma_{2k+1}\}_{k \geq 1} \leftrightarrow \{p_{2k+1}\}_{k \geq 1}$ . Now, as  $\text{gr}_{\mathcal{B}}\mathfrak{g}^m$  is dual to  $\text{gr}^{\mathcal{B}}\mathcal{L}$ , the existence of relations in  $\mathfrak{bg}$  implies the existence of additional relations in  $\text{gr}^{\mathcal{B}}\mathcal{L}$ . To be precise, we must have that  $\dim \text{gr}_n^{\mathcal{B}}\mathcal{L}_N < \dim \langle \text{I}^a(w) | \deg_{\mathcal{B}}(w) = n, |w| = N \rangle_Q$ , where we take  $\text{I}^a(w)$  to be its image in  $\mathcal{L}$ . Then, by the proof of Theorem 7.4 in [6], we know that the right hand side has is spanned by  $\{\zeta^a(k_1, \dots, k_r)\}$ , where  $k_i \in \{3, 2\}$ , exactly  $n$   $k_i = 3$  and  $k_1 + \dots + k_r = N$ . In particular, it has a basis given by such  $\zeta^a(k_1, \dots, k_r)$  such that  $(k_1, \dots, k_r)$  is a Lyndon word with respect to the order  $3 < 2$ . This basis, called the Hoffman-Lyndon basis, forms a spanning set for  $\dim \text{gr}_n^{\mathcal{B}}\mathcal{L}_N$ . Thus

$$\dim \text{gr}_n^{\mathcal{B}}\mathcal{L}_N < \dim \langle \text{I}^a(w) | \deg_{\mathcal{B}}(w) = n, |w| = N \rangle_Q$$

implies that there is a sum of Hoffman-Lyndon elements of weight  $N$  with  $n$  threes that can be written as a sum of Hoffman-Lyndon elements of weight  $N$  with fewer threes. However, the Hoffman-Lyndon elements of weight  $N$  form a basis of  $\mathcal{L}_N$ , and thus no such relation can exist. Thus we must have that  $\mathcal{L} \equiv \text{gr}^{\mathcal{B}}\mathcal{L}$  as they have equal dimensions and hence  $\text{gr}_{\mathcal{B}}\mathfrak{g}^m \equiv \mathfrak{g}^m$ . This implies  $\text{gr}_{\mathcal{B}}\mathfrak{g}^m$  and  $\mathfrak{bg}$  are both freely generated and isomorphic. □

**Remark 3.18.** While both Brown’s  $\mathfrak{dg}$  and our  $\mathfrak{bg}$  have canonical generators, Theorem 3.17 tells us that  $\mathfrak{bg}$  is free, while there exist relations in  $\mathfrak{dg}$ , and hence ‘exceptional’ generators are needed, first appearing in depth four. These relations are shown to have a somewhat mysterious connection to modular forms by Pollack [29], and this has been further explored by Baumard and Schneps [3]. However, it is a computationally challenging task, and suggests that ‘depth graded’ multiple zeta values may not be the most natural choice of object to study.

### 3.3 Polynomial Representations

We now reframe this Lie algebra in terms of commutative polynomials, similarly to Brown [8][9] and Écalle [17], as follows.

Recall that Charlton shows that every word  $w \in \{e_0, e_1\}^\times$  can be written uniquely as a sequence of alternating blocks [10]. In doing so, he establishes a bijection

$$\begin{aligned} \text{bl} : \{e_0, e_1\}^\times \setminus \{\emptyset\} &\rightarrow \bigcup_{n=1}^\infty \{0, 1\} \times \mathbb{N}^n \\ w &\mapsto (\epsilon; l_1, l_2, \dots, l_n) \end{aligned}$$

where  $\epsilon$  defines the first letter of  $w$ , and  $l_1, \dots, l_n$  describe the length of the alternating blocks.

**Example 3.19.**

$$\begin{aligned} e_0 e_1 e_0 e_0 e_1 e_0 e_1 e_1 &\mapsto (0; 3, 4, 1) \\ e_1 e_1 e_0 e_1 e_0 e_1 e_1 e_0 e_0 &\mapsto (1; 1, 5, 2, 1) \end{aligned}$$

We can use this to define a vector space isomorphism by

$$\begin{aligned} \pi_{\text{bl}} : \mathbb{Q}\langle e_0, e_1 \rangle \setminus \{\mathbb{Q} \cdot 1\} &\rightarrow \bigoplus_{n=1}^\infty x_1 \mathbb{Q}[x_1, \dots, x_n] x_n \\ w &\mapsto x_1^{l_1} \dots x_n^{l_n} \end{aligned} \tag{3.1}$$

where  $\text{bl}(e_0 w e_1) = (0; l_1, \dots, l_n)$ .

In this formulation, a word of block degree  $n$  and weight  $N \geq 1$  is represented by a polynomial in  $n + 1$  variables of degree  $N + 2$ . From this point on, we shall freely identify elements of  $\mathfrak{bg}$  with their images under this isomorphism. We refer to the images as ‘block polynomials’.

**Proposition 3.20.** *The projections of the depth-signed  $\sigma_{2k+1} \in \mathfrak{g}^{\mathfrak{m}}$  onto their block degree one part are given by*

$$p_{2k+1}(x_1, x_2) = q_{2k+1}(x_1, x_2) - q_{2k+1}(x_2, x_1)$$

where

$$\begin{aligned} q_{2k+1}(x_1, x_2) &= \sum_{i=1}^k \left[ \binom{2k}{2i} - \left(1 - \frac{1}{2^{2k}}\right) \binom{2k}{2k+1-2i} \right] x_1^{2i+1} x_2^{2k+2-2i} \\ &\quad - 2x_1 x_2^{2k+2} \end{aligned}$$

and  $\sigma_{2k+1}$  have been normalised to correspond to  $\frac{(-1)^k}{2} \zeta(2k+1)$ .

*Proof.* We will compute the block degree 1 part of  $\sigma_{2k+1}$  consisting of terms containing an  $e_0^2$ . This will give  $q_{2k+1}$ . That  $p_{2k+1}(x_1, x_2) = q_{2k+1}(x_1, x_2) - q_{2k+1}(x_2, x_1)$  follows from duality. In terms of  $e_0, e_1$ , we have

$$q_{2k+1} = \sum_{i=0}^k c_i (e_1 e_0)^i e_0 (e_1 e_0)^{k-i}$$

where  $\zeta^{\mathfrak{m}}(\{2\}^{i-1}, 3, \{2\}^{k-i}) = \alpha c_i \zeta^{\mathfrak{m}}(2k+1) \pmod{\zeta^{\mathfrak{m}}(2)}$ , for  $i > 0$  and some  $\alpha \in \mathbb{Q}$ , and  $c_0$  is obtained via shuffle regularisation [6].

Shuffle regularisation of  $e_0 e_1 \dots e_0$  tells us that

$$c_0 + 2 \sum_{i=1}^k c_i = 0$$

Next, from the work of Zagier [35]

$$\zeta(\{2\}^a, 3, \{2\}^b) = 2 \sum_{r=1}^{a+b+1} (-1)^r \left[ \binom{2r}{2a+2} - \left(1 - \frac{1}{2^{2r}} \binom{2r}{2b+1}\right) \right] \zeta(\{2\}^{a+b-r+1}) \zeta(2r+1)$$

Brown then shows in [6] Theorem 4.3 that this lifts to an identity among motivic multiple zeta values. Considered modulo  $\zeta^{\mathfrak{m}}(2)$ , we find

$$\zeta^{\mathfrak{m}}(\{2\}^{i-1}, 3, \{2\}^{k-i}) = 2(-1)^k \left[ \binom{2k}{2i} - \left(1 - \frac{1}{2^{2k}} \binom{2k}{2k+1-2i}\right) \right] \zeta^{\mathfrak{m}}(2k+1)$$

and thus we can take  $c_i = \left[ \binom{2k}{2i} - \left(1 - \frac{1}{2^{2k}} \binom{2k}{2k+1-2i}\right) \right]$  for  $i > 0$ . The result then follows.  $\square$

Computing these sums explicitly, we find that

**Theorem 3.21.**

$$p_{2k+1}(x_1, x_2) = x_1 x_2 (x_1 - x_2) \left( \frac{(1 - 2^{2k+1})(x_1 + x_2)^{2k} - (x_1 - x_2)^{2k}}{2^{2k}} \right)$$

With this in mind, we can provide a characterisation of these generators in terms of polynomial equations.

**Corollary 3.22.** *The polynomial  $p_{2k+1}(x_1, x_2)$  is, up to rescaling, the unique homogeneous polynomial  $p(x_1, x_2)$  of degree  $2k+3$  such that*

$$p(x_1, 0) = p(0, x_2) = p(x_1, x_2) + p(x_2, x_1) = 0$$

and, defining  $r(x_1, x_2) := \frac{p(x_1, x_2)}{x_1 x_2 (x_1 - x_2)}$ , satisfying

$$r(0, x) = r(x, -x)$$

and

$$\left( \frac{\partial}{\partial x_1} \right)^2 r(x_1, x_2) = \left( \frac{\partial}{\partial x_2} \right)^2 r(x_1, x_2)$$

*Proof.* The condition  $p(x_1, 0) = p(0, x_2) = p(x_1, x_2) + p(x_2, x_1) = 0$  suggests we can write  $p(x_1, x_2) = x_1 x_2 (x_1 - x_2) r(x_1, x_2)$ . Letting  $u = x_1 + x_2$ , and  $v = x_1 - x_2$ , we can rewrite

$$\left( \frac{\partial}{\partial x_1} \right)^2 r(x_1, x_2) = \left( \frac{\partial}{\partial x_2} \right)^2 r(x_1, x_2) \leftrightarrow \frac{\partial^2 r}{\partial u \partial v}(u, v) = 0$$

which has polynomial solution, homogeneous of degree  $(2k+3) - 3 = 2k$

$$r(u, v) = \alpha u^{2k} + \beta v^{2k}$$

and thus

$$r(x_1, x_2) = \alpha (x_1 + x_2)^{2k} + \beta (x_1 - x_2)^{2k}$$

Finally the condition

$$r(0, x) = 2r(x, -x)$$

gives

$$(\alpha + \beta)x^{2k} = 2^{2k+1}\beta x^{2k}$$

and hence

$$\alpha = -(1 - 2^{2k+1})\beta$$

giving the desired result.  $\square$

We can provide an exact polynomial formula for the Ihara action. Recall that we have chosen  $\mathfrak{g}^m$  to differ from Brown's by sending  $e_1 \mapsto -e_1$ , and so this is only accurate for 'depth-signed' elements. We delay the proof of this until later.

**Theorem 3.23.** *For (depth signed) elements of the motivic Lie algebra, the Ihara action is given at the level of block-polynomials by*

$$\begin{aligned} (f \circ g)(x_1, \dots, x_{m+n-1}) &= (-1)^{(m+1)(n+1)} \sum_{i=1}^n \frac{f(x_i, x_{i+1}, \dots, x_{i+m-1})}{x_i - x_{i+m-1}} \\ &\times \left( \frac{1}{x_i} g(x_1, \dots, x_{i-1}, x_i, x_{i+m}, \dots, x_{m+n-1}) \right. \\ &\left. - \frac{1}{x_{i+m-1}} g(x_1, \dots, x_{i-1}, x_{i+m-1}, \dots, x_{m+n-1}) \right) \end{aligned} \quad (3.2)$$

### 3.4 Relations arising in the polynomial representation

We find several relations arising naturally in the polynomial representation, preserved by the Ihara action, and dual to relations in  $\text{gr}_{\mathcal{B}}$ . We start by showing that duality is indeed preserved by our formula.

**Proposition 3.24.** *For all  $f(x_1, \dots, x_n) \in \mathfrak{bg}$*

$$f(x_1, \dots, x_n) = (-1)^{n+1} f(x_n, \dots, x_1)$$

*Proof.* It suffices to show that this holds for  $p_{2k+1}$ , and that, if this holds for  $f, g \in \mathfrak{bg}$ , then it

holds for  $f \circ g$ . The former holds by definition of  $p_{2k+1}$ . To see the latter, note that

$$\begin{aligned}
(f \circ g)(x_{m+n-1}, \dots, x_1) &= (-1)^{(m+1)(n+1)} \sum_{i=1}^n \frac{f(x_{m+n-i}, x_{m+n-i-1}, \dots, x_{n+1-i})}{x_{m+n-i}^2 - x_{n+1-i}^2} \\
&\quad \times \left( \left(1 + \frac{x_{n+1-i}}{x_{m+n-i}}\right) g(x_{m+n-1}, \dots, x_{m+n-i+1}, x_{m+n-i}, x_{n-i}, \dots, x_1) \right. \\
&\quad \left. - \left(1 + \frac{x_{m+n-i}}{x_{n+1-i}}\right) g(x_{m+n-1}, \dots, x_{m+n-i+1}, x_{n+1-i}, \dots, x_1) \right) \\
&= (-1)^{(m+1)(n+1)} \sum_{i=1}^n (-1)^m \frac{f(x_{n+1-i}, x_{n+2-1}, \dots, x_{m+n-i})}{x_{n+1-i}^2 - x_{m+n-i}^2} \\
&\quad \times \left( (-1)^{n+1} \left(1 + \frac{x_{n+1-i}}{x_{m+n-i}}\right) g(x_1, \dots, x_{n-i}, x_{m+n-i}, x_{m+n-i}, \dots, x_{m+n-1}) \right. \\
&\quad \left. - (-1)^{n+1} \left(1 + \frac{x_{m+n-i}}{x_{n+1-i}}\right) g(x_1, \dots, x_{n+1-i}, x_{m+n-i+1}, \dots, x_{m+n-1}) \right) \\
&= (-1)^{m+n} (-1)^{(m+1)(n+1)} \sum_{i=1}^n \frac{f(x_{n+1-i}, x_{n+2-1}, \dots, x_{m+n-i})}{x_{n+1-i}^2 - x_{m+n-i}^2} \\
&\quad \times \left( \left(1 + \frac{x_{m+n-i}}{x_{n+1-i}}\right) g(x_1, \dots, x_{n+1-i}, x_{m+n-i+1}, \dots, x_{m+n-1}) \right. \\
&\quad \left. - \left(1 + \frac{x_{n+1-i}}{x_{m+n-i}}\right) g(x_1, \dots, x_{n-i}, x_{m+n-i}, x_{m+n-i}, \dots, x_{m+n-1}) \right) \\
&= (-1)^{m+n} (f \circ g)(x_1, \dots, x_{m+n-1})
\end{aligned}$$

and hence the duality relation is preserved by the Ihara bracket.  $\square$

We can similarly prove Charlton's cyclic insertion conjecture, up to terms of lower block degree. While this has been verified in upcoming work due to Hirose-Sato, in this formulation, it is merely a consequence of the Ihara action, allowing for a significantly simpler proof. However, we will instead show that a more general relation holds, of which cyclic insertion is a corollary. These are the 'block shuffle' relations.

**Definition 3.25.** For any  $1 \leq r \leq n$ , define the shuffle set

$$\text{Sh}_{n,r} = \{\sigma \in \mathcal{S}_n \mid \sigma^{-1}(1) < \dots < \sigma^{-1}(r); \sigma^{-1}(r+1) < \dots < \sigma^{-1}(n)\}$$

Then, for any  $f \in \mathbb{Q}[x_1, \dots, x_n]$ , define

$$f(x_1 \dots x_r \sqcup x_{r+1} \dots x_n) := \sum_{\sigma \in \text{Sh}_{n,r}} f(x_{\sigma(1)}, x_{\sigma(2)}, \dots, x_{\sigma(n)})$$

**Theorem 3.26.** For any  $f(x_1, \dots, x_n) \in \mathfrak{bg}$ , and any  $1 \leq r < n$ , we have

$$f(x_1 x_2 \dots x_r \sqcup x_{r+1} \dots x_n) = 0$$

*Proof.* For  $p_{2k+1}$ , this is equivalent to  $p(x_1, x_2) + p(x_2, x_1) = 0$ , given by Proposition 3.24. Then, as the Ihara action is associative, it in fact suffices to show that

$$(f \circ g)(x_1 \dots x_r \sqcup x_{r+1} \dots x_{n+1}) = 0$$

for all  $f = p_{2k+1}$ ,  $g \in \mathfrak{bg}$ .

We write  $(f \circ g)(x_1 \dots x_r \sqcup x_{r+1} \dots x_{n+1})$  as

$$\sum_{\sigma \in \text{Sh}_{n+1,r}} \sum_{i=1}^n \frac{f(x_{\sigma(i)}, x_{\sigma(i+1)})}{x_{\sigma(i)} - x_{\sigma(i+1)}} \times \left( \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(i)}, x_{\sigma(i+2)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(i)}} - \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(i-1)}, x_{\sigma(i+1)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(i+1)}} \right)$$

This sum splits as follows

$$\begin{aligned} & \sum_{\sigma \in \text{Sh}_{n+1,r}} \sum_{i=1}^{r-1} \frac{f(x_{\sigma(i)}, x_{\sigma(i+1)})}{x_{\sigma(i)} - x_{\sigma(i+1)}} \times \\ & \left( \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(i)}, x_{\sigma(i+2)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(i)}} - \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(i-1)}, x_{\sigma(i+1)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(i+1)}} \right) \\ & + \sum_{\sigma \in \text{Sh}_{n+1,r}} \sum_{i=r+1}^n \frac{f(x_{\sigma(i)}, x_{\sigma(i+1)})}{x_{\sigma(i)} - x_{\sigma(i+1)}} \times \\ & \left( \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(i)}, x_{\sigma(i+2)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(i)}} - \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(i-1)}, x_{\sigma(i+1)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(i+1)}} \right) \\ & + \sum_{\substack{\sigma \in \text{Sh}_{n+1,r} \\ \text{such that} \\ \{\sigma(r), \sigma(r+1)\} \neq \{r, r+1\}}} \frac{f(x_{\sigma(r)}, x_{\sigma(r+1)})}{x_{\sigma(r)} - x_{\sigma(r+1)}} \times \\ & \left( \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(r)}, x_{\sigma(r+2)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(r)}} - \frac{g(x_{\sigma(1)}, \dots, x_{\sigma(r-1)}, x_{\sigma(r+1)}, \dots, x_{\sigma(n+1)})}{x_{\sigma(r+1)}} \right) \end{aligned}$$

Denote the first sum by  $A$ , the second by  $B$ , and the third by  $C$ . Now, this sum can be written uniquely as

$$\sum_{1 \leq k < l \leq n+1} \frac{f(x_k, x_l)}{x_k - x_l} \left( \frac{G_{k,l}}{x_k} - \frac{H_{k,l}}{x_l} \right)$$

where  $G_{k,l}, H_{k,l}$  are polynomials related by swapping  $x_k \leftrightarrow x_l$ . We have 4 cases to consider

1.  $l \leq r$
2.  $k \geq r+1$
3.  $k < r < r+1 < l$
4.  $k = r = l-1$

In the first case,  $A, B$  only contribute non-zero terms if  $l = k+1$ , while  $C$  only contributes if  $l > k+1$ . Thus, denoting by  $\Phi_k(\sigma, i)$  the condition  $\{\sigma(i) = k, \sigma(i+1) = k+1\}$ , we have

$$\begin{aligned} G_{k,k+1} &= \sum_{k \leq i < r} \sum_{\substack{\sigma \in \text{Sh}_{n+1,r} \\ \text{such that } \Phi_k(\sigma, i)}} g(x_{\sigma(1)}, \dots, x_{\sigma(i-1)}, x_k, x_{\sigma(i+2)}, \dots, x_{\sigma(n+1)}) \\ &+ \sum_{i > r} \sum_{\substack{\sigma \in \text{Sh}_{n+1,r} \\ \text{such that } \Phi_k(\sigma, i)}} g(x_{\sigma(1)}, \dots, x_{\sigma(i-1)}, x_k, x_{\sigma(i+2)}, \dots, x_{\sigma(n+1)}) \\ &+ \sum_{\substack{\sigma \in \text{Sh}_{n+1,r} \\ \text{such that } \Phi_k(\sigma, r)}} g(x_{\sigma(1)}, \dots, x_{\sigma(i-1)}, x_k, x_{\sigma(i+2)}, \dots, x_{\sigma(n+1)}) \end{aligned}$$

Let  $P(\sigma, r)$  denote the condition

$$\{\sigma^{-1}(1) < \dots < \sigma^{-1}(r); \sigma^{-1}(r+1) < \dots < \sigma^{-1}(n+1)\}$$

Then, this is a sum over the set of permutations

$$\cup_{k \leq i < r} \{\sigma | \Phi_k(\sigma, i) \text{ and } P(\sigma, r)\} \cup \cup_{i > r} \{\sigma | \Phi_k(\sigma, i) \text{ and } P(\sigma, r)\}$$

which is clearly in bijection with a set of shuffles of  $[n+1] \setminus \{k+1\}$ , and so the contribution is 0 by induction.

Then, if  $l > k+1$ , we find that the non-zero terms in

$$\frac{f(x_k, x_l)}{x_k - x_l} \left( \frac{G_{k,l}}{x_k} - \frac{H_{k,l}}{x_l} \right)$$

due to permutations with  $\sigma(r) = k, \sigma(r+1) = l$  cancel with those due to  $\sigma(r) = l, \sigma(r+1) = k$ . Thus, in this case,

$$\frac{f(x_k, x_l)}{x_k - x_l} \left( \frac{G_{k,l}}{x_k} - \frac{H_{k,l}}{x_l} \right) = 0$$

The second case,  $k \geq r+1$ , is similar. In the third case, every term due to a permutation with  $\sigma(i) = k, \sigma(i+1) = l$  cancels with the term due to the permutation  $\tau_{k,l} \circ \sigma$ , where  $\tau_{k,l}$  is the transposition  $(k, l)$ .

Finally, in the fourth case, our sum splits into a sum over the following sets

$$\cup_{i < r} \{\sigma \in \text{Sh}_{n+1,r} | \sigma(i) = r, \sigma(i+1) = r+1\}$$

$$\cup_{i > r} \{\sigma \in \text{Sh}_{n+1,r} | \sigma(i) = r, \sigma(i+1) = r+1\}$$

$$\cup_{i < r} \{\sigma \in \text{Sh}_{n+1,r} | \sigma(i) = r+1, \sigma(i+1) = r\}$$

$$\cup_{i > r} \{\sigma \in \text{Sh}_{n+1,r} | \sigma(i) = r+1, \sigma(i+1) = r\}$$

all of which must be empty due to the order preserving property of shuffle permutations. Thus,

$$(f \circ g)(x_1 \dots x_r \sqcup x_{r+1} \dots x_{n+1}) = 0$$

□

**Corollary 3.27.** *For any finite sequence of integers  $l_1, \dots, l_n$ , and any  $1 \leq r < n$ , we have*

$$\sum_{\sigma \in \text{Sh}_{n,r}} I^{\text{bl}}((l_{\sigma(1)}, \dots, l_{\sigma(n)}) = 0$$

when considered modulo products.

*Proof.* Using Theorem 3.17, we can consider  $\mathfrak{bg}$  as the dual Lie algebra to the graded Lie coalgebra of indecomposables  $\text{gr}_{\mathcal{B}}\mathcal{L}$ , and hence relations among the coefficients of elements of  $\mathfrak{bg}$  induce relations among elements of  $\text{gr}_{\mathcal{B}}\mathcal{L}$ . Specifically, we define a  $\mathbb{Q}$ -linear pairing

$$\langle I^{\text{bl}}(l_1, \dots, l_n) | x_1^{k_1} \dots x_m^{k_m} \rangle := \delta_{l_1, k_1} \dots \delta_{l_n, k_n}$$

where  $I^{\text{bl}}(l_1, \dots, l_n)$  is the image of  $I^{\text{b}}(l_1, \dots, l_n)$  in  $\text{gr}_{\mathcal{B}}\mathcal{L}$ , we have that  $R$  is a relation in  $\text{gr}_{\mathcal{B}}\mathcal{L}$  if and only if  $\langle R | f \rangle = 0$  for all  $f \in \mathfrak{bg}$ . Hence, as  $f(x_1 x_2 \dots x_r \sqcup x_{r+1} \dots x_n) = 0$  for all  $f \in \mathfrak{bg}$ , we must have that

$$\sum_{\sigma \in \text{Sh}_{n,r}} I^{\text{bl}}((l_{\sigma(1)}, \dots, l_{\sigma(n)}) = 0$$

□

**Corollary 3.28** (Block graded cyclic insertion). *The cyclic sum*

$$\sum_{\sigma \in C_n} I^{\text{bl}}(l_{\sigma(1)}, l_{\sigma(2)}, \dots, l_{\sigma(n)}) = 0$$

*Proof.* It suffices to show that

$$\sum_{\sigma \in C_n} f(x_{\sigma(1)}, x_{\sigma(2)}, \dots, x_{\sigma(n)}) = 0$$

for all  $f \in \mathfrak{bg}$ .

Suppose  $f \in \mathfrak{bg}$ . Then, Theorem 3.26 implies that the image of  $f$  under the following vector space isomorphism

$$\begin{aligned} \bigoplus_{n=0}^{\infty} \mathbb{Q}[x_1, \dots, x_n] &\xrightarrow{\sim} \mathbb{Q}\langle z_1, z_2, z_3, \dots \rangle \\ x_1^{i_1} x_2^{i_2} \dots x_n^{i_n} &\mapsto z_{i_1} z_{i_2} \dots z_{i_n} \end{aligned} \quad (3.3)$$

lies in  $\text{Lie}[z_1, z_2, \dots]$ . In particular, the image lies in the span of elements of degree at least 2. Now, we define a linear map  $\mathcal{C} : \mathbb{Q}\langle z_1, z_2, \dots \rangle \rightarrow \mathbb{Q}\langle z_1, z_2, \dots \rangle$  by

$$\mathcal{C}(z_{i_1} z_{i_2} \dots z_{i_n}) = \sum_{\sigma \in C_n} z_{i_{\sigma(1)}} z_{i_{\sigma(2)}} \dots z_{i_{\sigma(n)}}$$

for a word of length  $n$ . Thus, it suffices to show that  $\mathcal{C}(Z) = 0$  for all  $Z \in \text{Lie}[z_1, z_2, \dots]$  of degree at least 2.

As, for any monomials  $X, Y \in \{z_1, z_2, \dots\}$  of degree  $k, n - k$  respectively, we have  $[X, Y] = XY - \sigma(XY)$ , for some  $\sigma \in C_n$  acting by cyclic rotations on words of length  $n$ . Thus

$$\mathcal{C}([X, Y]) = \mathcal{C}(XY) - \mathcal{C}(\sigma(XY)) = \mathcal{C}(XY) - \mathcal{C}(XY) = 0$$

and so the image of any element of degree at least two in  $\text{Lie}[z_1, z_2, \dots]$  is zero, and hence

$$\sum_{\sigma \in C_n} f(x_{\sigma(1)}, x_{\sigma(2)}, \dots, x_{\sigma(n)}) = 0$$

□

**Remark 3.29.** As in this proof, it can be useful to consider  $\mathfrak{bg}$  as a subspace of  $\mathbb{Q}\langle z_1, z_2, z_3, \dots \rangle$ , considered as a Hopf algebra with the standard concatenation product, and a coproduct given by  $\Delta z_i = z_i \otimes 1 + 1 \otimes z_i$ . For example, Theorem 3.26 implies elements of  $\mathfrak{bg}$  are primitive for this coproduct, we immediately obtain Proposition 3.24 as a corollary, by considering the antipode map, the antihomomorphism  $z_i \mapsto -z_i$ . This is an idea we will explore further in section 3.11

### 3.5 Shuffle Regularisation

While the double shuffle relations among iterated integrals are not, in general, compatible with the block filtration, we find that the regularisation relation, obtained by shuffling with an element of weight 1, is.

**Theorem 3.30.** *Let  $\pi_1$  denote the projection map onto weight 1  $\mathbb{Q}\langle e_0, e_1 \rangle \rightarrow \mathbb{Q}e_0 \oplus \mathbb{Q}e_1$ , and let  $\Delta : \mathbb{Q}\langle e_0, e_1 \rangle \rightarrow \mathbb{Q}\langle e_0, e_1 \rangle \otimes \mathbb{Q}\langle e_0, e_1 \rangle$  be the coproduct defined by  $\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i$ . The map  $\Delta_1 := (\pi_1 \otimes \text{id})\Delta$  is compatible with the block filtration*

$$\Delta_1 \mathcal{B}^n \mathbb{Q}\langle e_0, e_1 \rangle \subset \mathcal{B}^1 \mathbb{Q}\langle e_0, e_1 \rangle \otimes \mathcal{B}^{n-1} \mathbb{Q}\langle e_0, e_1 \rangle$$

*Proof.* For  $w \in \mathbb{Q}\langle e_0, e_1 \rangle$  every term in  $\Delta_1(w)$  is of the form  $e_i \otimes \bar{w}$  for  $i \in \{0, 1\}$ ,  $\bar{w}$  obtained from  $w$  by omitting a letter. The left hand side is of block degree 1. The right hand side is either of higher block degree, if the omitted letter was internal to a block, or of block degree 1 lower than  $w$ , if the omitted letter was at the beginning or end of a block.  $\square$

Thus, we can take the associated graded map of  $\Delta_1$  to obtain

**Corollary 3.31.**  $gr_{\mathcal{B}}(\Delta_1)(\mathfrak{bg}) = 0$

*Proof.* This follows from the work of Brown [6] and Racinet [30], as any element  $\psi \in \mathfrak{g}^m$  satisfies  $\Delta(\psi) = 0$ .  $\square$

In low degree, we can translate this to a statement about elements of  $\mathfrak{bg}$  considered as block polynomials.

**Example 3.32.** For  $f(x_1, x_2) \in \mathfrak{bg}$  and  $g(x_1, x_2, x_3) \in \mathfrak{bg}$ , we have

$$\begin{aligned} x \frac{\partial f}{\partial x_1}(0, x) &= f(x, -x) \\ yz \left( \frac{\partial g}{\partial x_1}(0, y, z) - \frac{\partial g}{\partial x_1}(0, y, -z) \right) &= y(g(y, z, -z) + g(-y, z, -z)) \\ &\quad + z(g(-y, y, -z) - g(-y, y, z)) \\ yz \left( \frac{\partial g}{\partial x_1}(0, y, z) + \frac{\partial g}{\partial x_1}(0, y, -z) + \frac{\partial g}{\partial x_2}(y, 0, z) + \frac{\partial g}{\partial x_2}(y, 0, -z) \right) &= y(g(y, z, -z) - g(-y, z, -z)) \\ &\quad - z(g(-y, y, -z) + g(-y, y, z)) \end{aligned}$$

**Lemma 3.33.** For  $f(x_1, x_2, \dots, x_n) \in \mathfrak{bg}$ , we can write

$$f(x_1, \dots, x_n) = x_1 \dots x_n (x_1 - x_n) r(x_1, \dots, x_n)$$

for some polynomial  $r \in \mathbb{Q}[x_1, \dots, x_n]$ .

*Proof.* We induct on the number of variables. For  $n = 2$ , this follows from Theorem 3.21. Now, suppose this factorisation holds for  $f(x_1, x_2), g(x_1, \dots, x_n) \in \mathfrak{bg}$ . We have

$$\begin{aligned} \{f, g\} &= \sum_{i=1}^n \frac{f(x_i, x_{i+1})}{x_i - x_{i+1}} \times \\ &\quad \left( \frac{1}{x_i} g(x_1, \dots, x_i, x_{i+2}, \dots, x_{n+1}) - \frac{1}{x_{i+1}} g(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{n+1}) \right) \\ &\quad - g(x_1, \dots, x_n) \left( \frac{1}{x_1} f(x_1, x_{n+1}) - \frac{1}{x_n} f(x_n, x_{n+1}) \right) \\ &\quad - g(x_2, \dots, x_{n+1}) \left( \frac{1}{x_2} f(x_1, x_2) - \frac{1}{x_{n+1}} f(x_1, x_{n+1}) \right) \end{aligned}$$

Applying our induction hypothesis, we find

$$\begin{aligned} \{f, g\} &= x_1 \dots x_{n+1} r_f(x_1, x_2) \times \\ &\quad ((x_1 - x_{n+1}) r_g(x_1, x_3, \dots, x_{n+1}) - (x_2 - x_{n+1}) r_g(x_2, \dots, x_{n+1})) \\ &\quad + \sum_{i=2}^{n-1} x_1 \dots x_{n+1} (x_1 - x_{n+1}) r_f(x_i, x_{i+1}) \times \\ &\quad (r_g(x_1, \dots, x_i, x_{i+2}, \dots, x_{n+1}) - r_g(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{n+1})) \\ &\quad + x_1 \dots x_{n+1} r_f(x_n, x_{n+1}) \times \\ &\quad ((x_1 - x_n) r_g(x_1, \dots, x_n) - (x_1 - x_{n+1}) r_g(x_1, \dots, x_{n-1}, x_{n+1})) \\ &\quad - x_1 \dots x_{n+1} r_g(x_1, \dots, x_n) ((x_1 - x_{n+1}) r_f(x_1, x_{n+1}) - (x_n - x_{n+1}) r_f(x_n, x_{n+1})) \\ &\quad - x_1 \dots x_{n+1} r_g(x_2, \dots, x_{n+1}) ((x_1 - x_2) r_f(x_1, x_2) - (x_1 - x_{n+1}) r_f(x_1, x_{n+1})) \end{aligned}$$

Considering only the terms not immediately divisible by  $x_1 \dots x_{n+1}(x_1 - x_{n+1})$ , we reduce the problem to showing that

$$\begin{aligned}
& -x_1 \dots x_{n+1}(x_2 - x_{n+1})r_f(x_1, x_2)r_g(x_2, \dots, x_{n+1}) \\
& +x_1 \dots x_{n+1}(x_1 - x_n)r_f(x_n, x_{n+1})r_g(x_1, \dots, x_n) \\
& +x_1 \dots x_{n+1}(x_n - x_{n+1})r_f(x_n, x_{n+1})r_g(x_1, \dots, x_n) \\
& -x_1 \dots x_{n+1}(x_1 - x_2)r_f(x_1, x_2)r_g(x_2, \dots, x_{n+1}) \\
& = -x_1 \dots x_{n+1}(x_1 - x_{n+1})r_f(x_1, x_2)r_g(x_2, \dots, x_{n+1}) \\
& +x_1 \dots x_{n+1}(x_1 - x_{n+1})r_f(x_n, x_{n+1})r_g(x_1, \dots, x_n)
\end{aligned}$$

is divisible by  $x_1 \dots x_{n+1}(x_1 - x_{n+1})$ , and so we are done.  $\square$

**Definition 3.34.** For  $f(x_1, \dots, x_n) \in \mathfrak{bg}$ , define the reduced block polynomial to be

$$r(x_1, \dots, x_n) := \frac{f(x_1, \dots, x_n)}{x_1 \dots x_n(x_1 - x_n)}$$

Define  $\mathfrak{rbg}$  to be the bigraded  $\mathbb{Q}$ -vector space of reduced block polynomials.

**Remark 3.35.** It may be useful to recall how the various degrees we assign to motivic iterated integrals relate to the reduced block polynomials. A reduced block polynomial  $r(x_1, x_2, \dots, x_n)$  of degree  $N$  corresponds to elements of weight  $N + n - 1$  and block degree  $n - 1$ .

### 3.6 The dihedral action

As an immediate corollary to Proposition 3.24 we obtain:

**Lemma 3.36.** For all  $r(x_1, \dots, x_n) \in \mathfrak{rbg}$

$$r(x_n, \dots, x_1) = (-1)^n r(x_1, \dots, x_n)$$

**Definition 3.37.** We define a Lie algebra structure on  $\mathfrak{rbg}$  via the Lie bracket

$$\{r_1, r_2\}(x_1, \dots, x_{m+n-1}) := \frac{\{f_1, f_2\}(x_1, \dots, x_{m+n-1})}{x_1 \dots x_{m+n-1}(x_1 - x_{m+n-1})}$$

for  $r_1(x_1, \dots, x_m) = \frac{f_1(x_1, \dots, x_m)}{x_1 \dots x_m(x_1 - x_m)}$ ,  $r_2(x_1, \dots, x_n) = \frac{f_2(x_1, \dots, x_n)}{x_1 \dots x_n(x_1 - x_n)} \in \mathfrak{rbg}$ . We call this the reduced Ihara bracket. It produces a polynomial of degree  $\deg(r_1) + \deg(r_2)$ .

We can explicitly compute this, and in the case of  $r_1 = r_1(x_1, x_2)$ , we obtain a particularly nice formula.

**Proposition 3.38.** For  $r(x_1, x_2)$ ,  $q(x_1, \dots, x_{n-1}) \in \mathfrak{rbg}$ , the reduced Ihara bracket is given by

$$\{r, q\}(x_1, \dots, x_n) = \sum_{i=1}^n r(x_i, x_i + 1)(q(x_1, \dots, x_i, x_{i+2}, \dots, x_n) - q(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n))$$

where we consider indices modulo  $n$ .

**Corollary 3.39.**

$$r(x_1, \dots, x_n) = r(x_2, \dots, x_n, x_1)$$

for  $r(x_1, \dots, x_n) \in \mathfrak{rbg}$ .

*Proof.* This follows from a simple induction argument, using Lemma 3.36 as our base case, and the natural cyclic symmetry in Proposition 3.38.  $\square$

**Remark 3.40.** Corollary 3.28 follows as an immediate corollary to this invariance.

With this cyclic invariance, we can write down the general case of the reduced Ihara bracket quite succinctly.

**Corollary 3.41.** *For  $r(x_1, \dots, x_m), q(x_1, \dots, x_n) \in \mathbf{rbg}$ , the reduced Ihara bracket is given by*

$$\begin{aligned} \{r, q\}(x_1, \dots, x_{m+n-1}) = & \sum_{i=1}^{m+n-1} r(x_i, \dots, x_{i+m-1}) (q(x_{i+2}, \dots, x_{m+n-1}, x_1, \dots, x_i) \\ & - q(x_{i+1}, \dots, x_{m+n-1}, x_1, \dots, x_{i-1})) \end{aligned}$$

where the indices are considered modulo  $m + n - 1$ .

Thus, we have an action of the dihedral group on  $\mathbf{rbg}$ , restricting to either the trivial or sign representation on the block graded parts.

### 3.7 A Differential relation

We additionally obtain a differential relation, generalising the differential relation defining the generators of  $\mathbf{bg}$ .

**Definition 3.42.** For  $n \geq 2$ , define the differential operator

$$D_n : \mathbb{Q}[x_1, \dots, x_n] \rightarrow \mathbb{Q}[x_1, \dots, x_n]$$

by

$$D_n := \prod_{i_1, \dots, i_{n-1} \in \{0,1\}} \left( \frac{\partial}{\partial x_1} + (-1)^{i_1} \frac{\partial}{\partial x_2} + \dots + (-1)^{i_{n-1}} \frac{\partial}{\partial x_n} \right)$$

**Theorem 3.43.**

$$D_n r(x_1, \dots, x_n) = 0$$

for all  $r(x_1, \dots, x_n) \in \mathbf{rbg}$

*Proof.* We induct on  $n$ . For  $n = 2$ , this follows from Corollary 3.22. Suppose this holds for  $q(x_1, \dots, x_n) \in \mathbf{rbg}$ .

Next define

$$I_n := \{M \in M_n(\mu_2) \mid M_{i,i} = 1, \frac{M_{i+1,j}}{M_{i,j}} = \frac{M_{i+1,j+1}}{M_{i,j+1}}\}$$

and

$$L_M := \sum_{i=1}^n M_{1,i} \frac{\partial}{\partial x_i} = \pm \sum_{i=1}^n M_{j,i} \frac{\partial}{\partial x_i}$$

Note that  $D_n = \prod_{M \in I_n} L_M$ , and thus we have, for  $r(x_1, x_2), q(x_1, \dots, x_n) \in \mathbf{rbg}$ ,

$$\begin{aligned} D_{n+1} \{r, q\}(x_1, \dots, x_{n+1}) &= \sum_{i=1}^n D_{n+1} (r(x_i, x_{i+1}) q(x_i, x_{i+2}, \dots, x_{i+n}) - r(x_i, x_{i+1}) q(x_{i+1}, x_{i+2}, \dots, x_{i+n})) \\ &= \sum_{i=1}^n \sum_{S \subset I_{n+1}} \left( \prod_{M \in S} L_M \right) r(x_i, x_{i+1}) \left( \prod_{M \in I_{n+1} \setminus S} L_M \right) q(x_i, x_{i+2}, \dots, x_{i+n}) \\ &\quad - \sum_{i=1}^n \sum_{S \subset I_{n+1}} \left( \prod_{M \in S} L_M \right) r(x_i, x_{i+1}) \left( \prod_{M \in I_{n+1} \setminus S} L_M \right) q(x_{i+1}, x_{i+2}, \dots, x_{i+n}) \end{aligned}$$

where we have used the cyclic invariance of  $\mathbf{rbg}$ , and consider indices modulo  $n + 1$ .

Next note that, if we denote by  $M[i_1, \dots, i_k]$  the submatrix of  $M$  obtained by restricting to rows and columns  $i_1, \dots, i_k$ , we see that  $L_M f(x_{i_1}, \dots, x_{i_k}) = L_{M[i_1, \dots, i_k]} f(x_{i_1}, \dots, x_{i_k})$ .

Now, if  $\{M[i, i+1] \mid M \in S\} = I_2$ , then  $(\prod_{M \in S} L_M) r(x_i, x_{i+1}) = 0$ . Otherwise, we must have  $M[i, i+1] = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$  for all  $M \in S$ , or  $M[i, i+1] = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$  for all  $M \in S$ . In the first case, we must have all  $M \in I_{n+1}$  with  $M[i, i+1] = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$  contained in  $I_{n+1} \setminus S$ , and similarly for the second case. In either case, this implies that

$$\{M[i, i+2, \dots, i+n] \mid M \in I_{n+1} \setminus S\} = \{M[i+1, \dots, i+n] \mid I_{n+1} \setminus S\} = I_n$$

and so

$$\left( \prod_{M \in I_{n+1} \setminus S} L_M \right) q(x_i, x_{i+2}, \dots, x_{i+n}) = \left( \prod_{M \in I_{n+1} \setminus S} L_M \right) q(x_{i+1}, x_{i+2}, \dots, x_{i+n}) = 0$$

Thus  $D_{n+1}\{r, q\} = 0$ .

□

**Remark 3.44.** Note that, in sufficiently high degree,  $r(x_1, \dots, x_n) \in \ker D_n$  is equivalent to  $r(x_1, \dots, x_n) \in \sum_{M \in I_n} \ker L_M$ . This second condition clearly holds for  $n = 2$ , and can easily be shown to be preserved by the Ihara bracket. Hence, we can rephrase Theorem 3.43 as the following statement:

$$r(x_1, \dots, x_n) \in \sum_{M \in I_n} \ker L_M \text{ for all } r(x_1, \dots, x_n) \in \mathbf{rbg}$$

As the kernel of  $L_M$  is spanned by elements of the form  $(x_1 \pm x_2)^{d_1} (x_2 \pm x_3)$ .

**Remark 3.45.** We have shown that, in block degree 1,  $\mathbf{bg}$  is isomorphic as a vector space to the bigraded vector space of homogeneous polynomials satisfying Theorem 3.26, Example 3.32, Lemma 3.33, and whose reduced forms satisfy Corollary 3.39 and Theorem 3.43. Note also that, as all these properties are preserved by the Ihara bracket, we obtain that  $\mathbf{bg}$  is a Lie subalgebra of the Lie algebra of homogeneous polynomials satisfying these properties. However, in block degree  $b$ , and weight  $w$ , we can only show that the dimension of the bigraded piece of the vector space of homogeneous polynomials satisfying these constraints is bounded above by  $Cw^{b-1}$  for some constant  $C$ .

### 3.8 Further Results in Block Degree 2

While we can uniquely described elements of  $\mathbf{bg}_1$  as solutions to a set of equations, in block degree 1, we can only bound the dimension above by something growing linearly in weight. However, we can exactly describe where the ambiguity lies. Let  $r(x_1, x_2, x_3) \in \mathbf{rbg}_2$ . Then we have that

$$\begin{aligned} r(x_1, x_2, x_3) &= r(x_2, x_3, x_1) = -r(x_3, x_2, x_1) \\ \frac{\partial^4 r}{\partial x_1^4} + \frac{\partial^4 r}{\partial x_2^4} + \frac{\partial^4 r}{\partial x_3^4} - 2 \frac{\partial^4 r}{\partial x_1^2 \partial x_2^2} - 2 \frac{\partial^4 r}{\partial x_2^2 \partial x_3^2} - 2 \frac{\partial^4 r}{\partial x_3^2 \partial x_1^2} &= 0 \end{aligned}$$

and that  $g(x_1, x_2, x_3) := x_1 x_2 x_3 (x_1 - x_3) r(x_1, x_2, x_3)$  satisfies the shuffle regularisation equations.

$$\begin{aligned}
yz \left( \frac{\partial g}{\partial x_1}(0, y, z) - \frac{\partial g}{\partial x_1}(0, y, -z) \right) &= y(g(y, z, -z) + g(-y, z, -z)) \\
&\quad + z(g(-y, y, -z) - g(-y, y, z)) \\
yz \left( \frac{\partial g}{\partial x_1}(0, y, z) + \frac{\partial g}{\partial x_1}(0, y, -z) + \frac{\partial g}{\partial x_2}(y, 0, z) + \frac{\partial g}{\partial x_2}(y, 0, -z) \right) &= y(g(y, z, -z) - g(-y, z, -z)) \\
&\quad - z(g(-y, y, -z) + g(-y, y, z))
\end{aligned}$$

Writing these relations in terms of  $r(x_1, x_2, x_3)$ , we find that these both reduce to

$$\frac{1}{2}(r(0, y, z) - r(0, y, -z)) = r(-y, y, z) - r(y, -z, z)$$

Observe that, considering the parity of the degrees of monomials, we must have that the totally even part of  $r$

$$r_e(x_1, x_2, x_3) := \frac{1}{4}(r(x_1, x_2, x_3) + r(-x_1, x_2, x_3) + r(x_1, x_2, -x_3) + r(-x_1, x_2, -x_3))$$

and the odd part of  $r$ ,  $r_o(x_1, x_2, x_3) := r(x_1, x_2, x_3) - r_e(x_1, x_2, x_3)$ , must both satisfy these equations separately. We claim that, if  $q(x_1, x_2, x_3)$  satisfies these equations, then there exists  $r(x_1, x_2, x_3) \in \mathbf{rbg}_2$  such that  $q_o(x_1, x_2, x_3) = r_o(x_1, x_2, x_3)$ . Equivalently, we have the following.

**Proposition 3.46.** *Let  $V_o^{2n} \subset \mathbb{Q}[x_1, x_2, x_3]$  be the space of homogeneous polynomials of degree  $2n$ , satisfying*

$$\begin{aligned}
q(x_1, x_2, x_3) &= q(x_2, x_3, x_1) = -q(x_3, x_2, x_1) \quad (1) \\
\frac{1}{2}(q(0, y, z) - q(0, y, -z)) &= q(-y, y, z) - q(y, -z, z) \quad (2) \\
\frac{\partial^4 q}{\partial x_1^4} + \frac{\partial^4 q}{\partial x_2^4} + \frac{\partial^4 q}{\partial x_3^4} - 2\frac{\partial^4 q}{\partial x_1^2 \partial x_2^2} - 2\frac{\partial^4 q}{\partial x_2^2 \partial x_3^2} - 2\frac{\partial^4 q}{\partial x_3^2 \partial x_1^2} &= 0 \quad (3) \\
q_e(x_1, x_2, x_3) &= 0 \quad (4)
\end{aligned}$$

and let  $d_2^{2n}$  be the dimension of the degree  $2n$  piece of  $\mathbf{rbg}_2$ , i.e. the dimension of the weight  $2n + 2$  part of  $\mathbf{bg}_2$ . Then  $\dim V_o^{2n} = d_2^{2n}$ .

*Proof.* We first note that  $d_2^{2n}$  is the number of independent Lie brackets  $\{p_{2k+1}, p_{2l+1}\}$  with  $2k + 2l + 2 = 2n + 2$ , with  $k, l > 1$ . This is precisely the number of positive integer solutions to  $k + l = n$  with  $1 < k < l$ . Thus  $d_2^{2n} = \lfloor \frac{n-1}{2} \rfloor$ .

Next, Equation (3) implies

$$\begin{aligned}
q(x_1, x_2, x_3) &= \sum_{i+j=2n} \alpha_{i,j}(x_1 - x_2)^i(x_2 - x_3)^j + \beta_{i,j}(x_1 + x_2)^i(x_2 - x_3)^j \\
&\quad + \gamma_{i,j}(x_1 - x_2)^i(x_2 + x_3)^j + \delta_{i,j}(x_1 + x_2)^i(x_2 + x_3)^j
\end{aligned}$$

Denoting by  $q_\star(x_1, x_2, x_3) = \frac{1}{4}(q(x_1, x_2, x_3) - q(-x_1, x_2, x_3) - q(x_1, x_2, -x_3) + q(-x_1, x_2, -x_3))$  the part of  $q$  that is odd in  $x_1, x_3$  and even in  $x_2$ , we can write

$$\begin{aligned}
q_\star(x_1, x_2, x_3) &= \sum_{\substack{i+j=2n \\ i,j>0}} \rho_{i,j}((x_1 - x_2)^i(x_2 - x_3)^j + (-1)^{i+1}(x_1 + x_2)^i(x_2 - x_3)^j \\
&\quad - (x_1 - x_2)^i(x_2 + x_3)^j + (-1)^i(x_1 + x_2)^i(x_2 + x_3)^j)
\end{aligned}$$

where  $\rho_{i,j} := \alpha_{i,j} + (-1)^{i+1}\beta_{i,j} - \gamma_{i,j} + (-1)^i\delta_{i,j}$ . As  $q(x_1, x_2, x_3) = -q(x_3, x_2, x_1)$ , the same holds for  $q_*(x_1, x_2, x_3)$  and thus  $\rho_{i,j} = -\rho_{j,i}$ .

Then, as  $q_e(x_1, x_2, x_3) = 0$ , and  $q(x_1, x_2, x_3) = q(x_2, x_3, x_1)$ , we must have

$$q(x_1, x_2, x_3) = q_*(x_1, x_2, x_3) + q_*(x_2, x_3, x_1) + q_*(x_3, x_1, x_2)$$

Thus,  $q$  is uniquely determined by  $q_*$ . We currently have  $n - 1$  free variables in  $q_*$ , so in order for  $\dim V_o^{2n}$  to be equal to  $\lfloor \frac{n-1}{2} \rfloor$ , we need Equation (2) to impose  $\lceil \frac{n-1}{2} \rceil$  independent constraints on the  $\rho_{i,j}$ .

Writing Equation (2) in terms of  $q_*(x_1, x_2, x_3)$ , we find that we must have

$$q_*(z, 0, y) = 2q_*(z, y, y) - 2q_*(y, z, z)$$

Evaluating the coefficient of  $y^k z^l$  in this equation we obtain

$$\rho_{l,k} = \sum_{\substack{0 \leq j \leq k \\ i+j=2n}} (-2)^j \binom{i}{l} \rho_{i,j} - \sum_{\substack{0 \leq j \leq l \\ i+j=2n}} (-2)^j \binom{i}{k} \rho_{i,j}$$

if  $k$  is odd, and  $0 = 0$  if  $k$  is even, or if  $k = l$ . As the coefficient of  $y^l z^k$  is just the negative of this, this gives us  $\lceil \frac{n-1}{2} \rceil$  equations, so it suffices to show that they are independent. As we are solving for rational  $\rho_{i,j}$ , it is sufficient to show that these equations are independent modulo 2. But, mod 2 we obtain

$$\rho_{l,k} \equiv 0 \pmod{2}$$

which are clearly independent. Hence, we have  $\lfloor \frac{n-1}{2} \rfloor$  free variables in  $q_*$  and this  $\dim V_o^{2n} = \lfloor \frac{n-1}{2} \rfloor = d_2^{2n}$ .  $\square$

### 3.9 Deriving the Ihara action formula

For elements of the double shuffle Lie algebra, the (linearised) Ihara action is given by the following [9]

**Proposition 3.47.** *For  $\sigma \in \text{Lie}[e_0, e_1]$ ,  $u \in \{e_0, e_1\}^\times$ , the linearised Ihara action is given recursively by*

$$\sigma \circ e_0^n e_1 u := e_0^n \sigma e_1 u - e_0^n e_1 \sigma^* u + e_0^n e_1 (\sigma \circ u) \quad (3.4)$$

where  $(a_1 \dots a_n)^* := (-1)^n a_n \dots a_1$ .

Translating the linearised Ihara action into the language of commutative variables, we find the following.

**Theorem 3.48.** *For  $f(x_1, \dots, x_m)$  the image of the block degree  $m - 1$  part of  $\sigma \in \text{Lie}[e_0, e_1]$ ,  $g \in \mathbb{Q}[x_1, \dots, x_n]$ , the linearised Ihara action is given by*

$$\begin{aligned} (f \circ g)(x_1, \dots, x_{m+n-1}) &= \sum_{i=1}^n (-1)^{(m+1)(i-1)} \frac{f(x_i, x_{i+1}, \dots, x_{i+m-1})}{x_i^2 - x_{i+m-1}^2} \\ &\quad \times \left( \left(1 + (-1)^{m+1} \frac{x_{i+m-1}}{x_i}\right) g(\bar{x}_1, \dots, \bar{x}_i, x_{i+m}, \dots, x_{m+n-1}) \right. \\ &\quad \left. - \left(1 + (-1)^{m+1} \frac{x_i}{x_{i+m-1}}\right) g(\bar{x}_1, \dots, \bar{x}_{i-1}, x_{i+m-1}, \dots, x_{m+n-1}) \right) \end{aligned}$$

where we define  $\bar{x}_i := (-1)^{m+1} x_i$ .

*Proof.* We start by writing, for  $u = u_1 \dots u_n \in \{e_0, e_1\}^\times$ ,

$$\sigma \circ u_1 \dots u_n = \epsilon_0 \sigma u_1 \dots u_n + \sum_{i=1}^n \epsilon_i u_1 \dots u_i \sigma u_{i+1} \dots u_n$$

where  $\epsilon_i \in \{0, \pm 1\}$  for each  $i$ . We first claim that  $\epsilon_i = 0$  if  $u_i = u_{i+1}$ . We take here  $u_0 = e_0$ , and  $u_{n+1} = e_1$ .

If  $u_i = u_{i+1} = e_0$ , then our recursive formula (3.4) shows  $\epsilon_i = 0$ , as  $\sigma$  does not ‘insert’ between adjacent  $e_0$ . If  $u_i = u_{i+1} = e_1$ , then our recursion gives us terms of the form

$$\dots + u_1 \dots u_{i-1} e_1 \sigma^* e_1 u_{i+2} \dots u_n + u_1 \dots u_{i-1} e_1 \sigma e_1 u_{i+2} \dots u_n + u_1 \dots u_{i-1} e_1 e_1 \sigma^* u_{i+2} \dots u_n + \dots$$

As, for  $\sigma \in \text{Lie}[e_0, e_1]$ ,  $\sigma + \sigma^* = 0$ , the terms corresponding to  $u_1 \dots u_i \sigma u_{i+1} \dots u_n$  cancel, giving us that  $\epsilon_i = 0$ .

Hence, our block-polynomial formula will consist of a sum over the blocks of  $u$ , each corresponding to the insertion of  $\sigma$  into a single block.

We will induct on the number of blocks in  $u$ . If  $u$  consists of a single block,  $u = (e_1 e_0)^k$ , and

$$\begin{aligned} \sigma \circ u &= \sigma(e_1 e_0)^k + e_1 \sigma^* e_0 (e_1 e_0)^{k-1} + e_1 e_0 \sigma (e_1 e_0)^{k-2} + e_1 e_0 e_1 \sigma^* e_0 (e_1 e_0)^{k-3} + \dots \\ &= \sum_{i=0}^k (e_1 e_0)^i \sigma (e_1 e_0)^{k-i} + (e_1 e_0)^i e_1 \sigma^* e_0 (e_1 e_0)^{k-1-i} \end{aligned}$$

Now, letting  $f(x_1, \dots, x_m)$  be the polynomial representating the block degree  $n$  part of  $\sigma$  and  $g(x_1) = x_1^{2k+2}$  be the polynomial representing  $u$ , this is equivalent to the statement that

$$\begin{aligned} (f \circ g)(x_1, \dots, x_m) &= \sum_{i=0}^k \left( \frac{x_1}{x_m} \right)^{2i} \frac{f(x_1, \dots, x_m) g(x_m)}{x_m^2} + (-1)^{m+1} \frac{x_1}{x_m} \sum_{i=0}^{k-1} \left( \frac{x_1}{x_m} \right)^{2i} \frac{f(x_1, \dots, x_m) g(x_m)}{x_m^2} \\ &= \frac{f(x_1, \dots, x_m)}{x_1^2 - x_m^2} \left( \left( \frac{x_1}{x_m} \right)^{2k+2} - 1 + (-1)^{m+1} \left( \frac{x_1}{x_m} \right)^{2k+1} - (-1)^{m+1} \frac{x_1}{x_m} \right) g(x_m) \\ &= \frac{f(x_1, \dots, x_m)}{x_1^2 - x_m^2} \left( g(x_1) - g(x_m) + (-1)^{m+1} \frac{x_m}{x_1} g(x_1) - (-1)^{m+1} \frac{x_1}{x_m} g(x_m) \right) \end{aligned}$$

which is precisely the result given by the formula.

Now suppose our formula is correct for words consisting of  $n - 1$  blocks, and let  $e_0 u e_1$  be a word consisting of  $n$  blocks  $e_0 u e_1 = b_1 \dots b_n$ , corresponding to the monomial  $g(x_1, \dots, x_n)$ . As we have merely appended a block onto the end of a word, the first  $n - 2$  terms of  $(f \circ g)$  will be given by our formula, by our induction hypothesis. To see this, consider  $(f \circ g_{alt})$ , where  $g_{alt}$  is the polynomial corresponding to the word  $e_0 u_{alt} e_1 = b_1 \dots b'_{n-1}$ . Here  $b'_{n-1}$  is the smallest block extending  $b_{n-1}$  and ending on  $e_1$ . The Ihara action of any  $\sigma \in \text{Lie}[e_0, e_1]$  on  $u$  and  $u_{alt}$  will produce terms that are identical upon swapping  $b_{n-1} b_n \leftrightarrow b'_{n-1}$  up to those terms in which  $\sigma$  inserts into  $b_{n-1} b_n$ . Indeed, they will agree under this swapping until we consider terms in which  $\sigma$  inserts beyond the end of  $b_{n-1}$ .

Thus, it suffices to show that the formula holds for a word  $e_0 u e_1 = b_1 b_2$  of block degree 1. We have 2 cases: the repeated letter in  $e_0 u e_1$  is  $e_0$ , or it is  $e_1$ .

In the first case,  $u = (e_1 e_0)^k e_0 (e_1 e_0)^l$  and

$$\begin{aligned} \sigma \circ u &= \sum_{i=0}^k (e_1 e_0)^i \sigma (e_1 e_0)^{k-i} e_0 (e_1 e_0)^l + \sum_{i=0}^{k-1} (e_1 e_0)^i e_1 \sigma^* e_0 (e_1 e_0)^{k-1-i} e_0 (e_1 e_0)^l \\ &\quad + \sum_{i=0}^l (e_1 e_0)^k e_0 (e_1 e_0)^i \sigma (e_1 e_0)^{l-i} + \sum_{i=0}^{l-1} (e_1 e_0)^k e_0 (e_1 e_0)^i e_1 \sigma^* e_0 (e_1 e_0)^{l-1-i} \end{aligned}$$

In terms of commutative polynomials, after summing the geometric series, we obtain

$$(f \circ g)(x_1, \dots, x_{m+1}) = \frac{f(x_1, \dots, x_m)}{x_1^2 - x_m^2} \left( \left( \frac{x_1}{x_m} \right)^{2k} - 1 + (-1)^{m+1} \left( \frac{x_1}{x_m} \right)^{2k+1} - (-1)^{m+1} \frac{x_1}{x_m} \right) g(x_m, x_{m+1}) \\ + \frac{f(x_2, \dots, x_{m+1})}{x_2^2 - x_{m+1}^2} \left( \left( \frac{x_2}{x_{m+1}} \right)^{2l+2} - 1 + (-1)^{m+1} \left( \frac{x_2}{x_{m+1}} \right)^{2l+1} - (-1)^{m+1} \frac{x_2}{x_{m+1}} \right) g(x_1, x_{m+1})$$

Simplifying, and noting that  $g(x_1, x_2) = x_1^{2k+1} x_2^{2l+2}$ , we obtain

$$(f \circ g)(x_1, \dots, x_{m+1}) = \frac{f(x_1, \dots, x_m)}{x_1^2 - x_m^2} \left( \frac{x_m}{x_1} g(x_1, x_m + 1) - g(x_m, x_m + 1) \right. \\ \left. + (-1)^{m+1} g(x_1, x_{m+1}) - (-1)^{m+1} \frac{x_1}{x_m} g(x_m, x_{m+1}) \right) \\ + \frac{f(x_2, \dots, x_{m+1})}{x_2^2 - x_{m+1}^2} (g(x_1, x_2) - g(x_1, x_{m+1}) \\ + (-1)^{m+1} \frac{x_{m+1}}{x_2} g(x_1, x_2) - (-1)^{m+1} \frac{x_2}{x_{m+1}} g(x_1, x_{m+1}))$$

Considering parity, and defining  $\bar{x}_i := (-1)^{m+1} x_i$ , we can rewrite this as

$$(f \circ g)(x_1, \dots, x_{m+1}) = (-1)^{(0)(m+1)} \frac{f(x_1, \dots, x_m)}{x_1^2 - x_m^2} \left( g(\bar{x}_1, x_{m+1}) + (-1)^{m+1} \frac{x_m}{x_1} g(\bar{x}_1, x_{m+1}) \right. \\ \left. - g(x_m, x_{m+1}) + (-1)^{m+1} \frac{x_m}{x_{m+1}} g(x_m, x_{m+1}) \right) \\ + (-1)^{m+1} \frac{f(x_2, \dots, x_{m+1})}{x_2^2 - x_{m+1}^2} \left( g(\bar{x}_1, \bar{x}_2) - (-1)^{m+1} \frac{x_{m+1}}{x_2} g(\bar{x}_1, \bar{x}_2) \right. \\ \left. - g(\bar{x}_1, x_{m+1}) + (-1)^{m+1} \frac{x_2}{x_{m+1}} g(\bar{x}_1, x_{m+1}) \right)$$

giving the desired formula. The second case follows similarly.

Hence, our general formula is

$$\begin{aligned}
(f \circ g)(x_1, \dots, x_{m+n-1}) &= \sum_{i=1}^{n-2} (-1)^{(m+1)(i-1)} \frac{f(x_i, x_{i+1}, \dots, x_{i+m-1})}{x_i^2 - x_{i+m-1}^2} \\
&\quad \times \left( (1 + (-1)^{m+1} \frac{x_{i+m-1}}{x_i}) g(\bar{x}_1, \dots, \bar{x}_i, x_{i+m}, \dots, x_{m+n-1}) \right. \\
&\quad \left. - (1 + (-1)^{m+1} \frac{x_i}{x_{i+m-1}}) g(\bar{x}_1, \dots, \bar{x}_{i-1}, x_{i+m-1}, \dots, x_{m+n-1}) \right) \\
&\quad \pm (-1)^{(m+1)(n-2)} \frac{f(x_{n-1}, \dots, x_{m+n-2})}{x_{n-1}^2 - x_{m+n-2}^2} \\
&\quad \times \left( (1 + (-1)^{m+1} \frac{x_{m+n-2}}{x_{n-1}}) g(\bar{x}_1, \dots, \bar{x}_{n-1}, x_{m+n-1}) \right. \\
&\quad \left. - (1 + (-1)^{m+1} \frac{x_{n-1}}{x_{m+n-2}}) g(\bar{x}_1, \dots, \bar{x}_{n-2}, x_{m+n-2}, x_{m+n-1}) \right) \\
&\quad \pm (-1)^{(m+1)(n-1)} \frac{f(x_n, \dots, x_{m+n-1})}{x_n^2 - x_{m+n-1}^2} \\
&\quad \times \left( (1 + (-1)^{m+1} \frac{x_{m+n-1}}{x_n}) g(\bar{x}_1, \dots, \bar{x}_n) \right. \\
&\quad \left. - (1 + (-1)^{m+1} \frac{x_n}{x_{m+n-1}}) g(\bar{x}_1, \dots, \bar{x}_{n-1}, x_{m+n-1}) \right)
\end{aligned}$$

where the sign of the final two summands agree. To fix this sign, we need only to consider the sign of the term corresponding to  $(\frac{x_{n-1}}{x_{m+n-2}})^2 \frac{f(x_{n-1}, \dots, x_{m+n-2}) g(\bar{x}_1, \dots, \bar{x}_{n-2}, x_{m+n-2}, x_{m+n-1})}{x_{m+n-2}^2}$ . This corresponds to inserting  $\sigma$  after the first two letters of the  $(n-1)$ -th block. This will be positive if this block starts with an  $e_1$  and have the same sign as  $(-1)^{m+1}$  otherwise. Let  $g(x_1, \dots, x_n) = x_1^{d_1} \dots x_n^{d_n}$ . Then, by Lemma 3.10 the  $(n-1)$ -th block starts with  $e_0$  if  $d_1 + \dots + d_{n-2} \equiv n-2 \pmod{2}$ , and  $e_1$  otherwise. Thus, the sign of the term corresponding to  $(\frac{x_{n-1}}{x_{m+n-2}})^2 \frac{f(x_{n-1}, \dots, x_{m+n-2}) g(\bar{x}_1, \dots, \bar{x}_{n-2}, x_{m+n-2}, x_{m+n-1})}{x_{m+n-2}^2}$  is  $(-1)^{(m-1)(1+d_1+\dots+d_{n-2}-n+2)}$ . Comparing this with our formula, we see that the final two terms must appear with a positive sign, giving the desired result.  $\square$

To obtain (3.2), we must translate this across into the ‘depth signed’ convention. Specifically, we must find the action of the map  $e_1 \mapsto -e_1$  in terms of commutative variables.

**Lemma 3.49.** *The automorphism  $\mathbb{Q}\langle e_0, e_1 \rangle \rightarrow \mathbb{Q}\langle e_0, e_1 \rangle$  given by  $e_1 \mapsto -e_1$ , is equivalent under the isomorphism (3.1) to the map*

$$\begin{aligned}
\mathbb{Q}[x_1, \dots, x_n] &\rightarrow \mathbb{Q}[x_1, \dots, x_n] \\
f(x_1, \dots, x_n) &\mapsto (-1)^{\lceil \frac{l}{2} \rceil} f(-x_1, x_2, \dots, (-1)^n x_n)
\end{aligned} \tag{3.5}$$

for  $f$  a homogeneous polynomial of degree  $l+2$ .

*Proof.* Note that it suffices to show that, for a word  $w$  of length  $l$  and depth  $d$ , with  $\pi_{\text{bl}}(w) = x_1^{d_1} \dots x_n^{d_n}$ , that this congruence holds

$$d \equiv \lceil \frac{l}{2} \rceil + d_1 + d_3 + \dots \pmod{2}.$$

We will induct on the number of blocks in  $e_0 w e_1$ . If  $e_0 w e_1$  consists of a single block, then  $e_0 w e_1 = (e_0 e_1)^{\frac{l}{2}+1}$ , and so  $d = \frac{l}{2}$ , and  $d_1 = l+2$ . Thus the result holds.

Suppose the result holds for  $w$  such that  $e_0 w e_1$  consists of  $n$  blocks. Let  $e_0 w e_1 = w' w_{d_{n+1}}$  be a word of length  $l+2$  and depth  $d+1$ , consisting of  $n+1$  blocks, where  $w_{d_{n+1}}$  is a single block of length  $d_{n+1}$  and  $w'$  is a word of length  $l'$  and depth  $d'$ . Suppose  $\pi_{\text{bl}}(w) = x_1^{d_1} \dots x_n^{d_n} x_{n+1}^{d_{n+1}}$ .

If  $l'$  is even, then  $w' = e_0 u e_1$  consists of  $n \equiv 1 \pmod{2}$  blocks, and  $d_{n+1}$  must be odd. So, by induction,

$$d' - 1 \equiv \frac{l' - 2}{2} + \sum_{1 \leq 2i+1 \leq n} d_{2i+1} \pmod{2}$$

Thus

$$\begin{aligned} d &= d' + \left\lceil \frac{d_{n+1}}{2} \right\rceil - 1 \\ &\equiv \frac{l' - 2}{2} + \sum_{1 \leq 2i+1 \leq n} d_{2i+1} \pmod{2} + \left\lceil \frac{d_{n+1}}{2} \right\rceil \pmod{2} \\ &\equiv \left\lceil \frac{l' + d_{n+1} - 2}{2} \right\rceil + \sum_{1 \leq 2i+1 \leq n+1} d_{2i+1} \pmod{2} \pmod{2} \\ &\equiv \left\lceil \frac{l}{2} \right\rceil + \sum_{1 \leq 2i+1 \leq n+1} d_{2i+1} \pmod{2} \pmod{2} \end{aligned}$$

And so the result holds. Similar considerations for  $l'$  odd prove the result in general.  $\square$

Applying this transformation, and simplifying, we obtain Proposition 3.23, giving the formula

$$\begin{aligned} (f \circ g)(x_1, \dots, x_{m+n-1}) &= \sum_{i=1}^n \frac{f(x_i, \dots, x_{i+m-1})}{x_i - x_{i+m-1}} \left( \frac{1}{x_i} g(x_1, \dots, x_i, x_{i+m}, \dots, x_{m+n-1}) \right. \\ &\quad \left. - \frac{1}{x_{i+m-1}} g(x_1, \dots, x_{i-1}, x_{i+m-1}, \dots, x_{m+n-1}) \right) \end{aligned}$$

### 3.10 Additional block graded relations

We can, similarly to Corollary 3.31, attempt to define graded analogues of existing relations among block graded multiple zeta values. For example, a weaker formulation of shuffle regularisation exists, obtained by composing  $\text{gr}_{\mathcal{B}}(\Delta_1)$  with projection onto the second component.

**Corollary 3.50.** *For  $f(x_1, \dots, x_n) \in \mathbf{bg}$*

$$\sum_{i=1}^{n-1} \frac{f(x_1, \dots, x_i, x_i, \dots, x_{n-1})}{x_i} = 0$$

Attempting similar with the stuffle equations, we find that it is difficult to encode stuffle relations as functional equations satisfied by elements of  $\mathbf{bg}$ . Instead, we return to direct computations with multiple zeta values. We first note that, for convergent MZVs, computation of block degree is a function of the arguments.

**Lemma 3.51.** *The block degree of  $\zeta^{\mathbf{m}}(n_1, \dots, n_k)$  is given by  $\sum_{i=1}^k |n_i - 2|$ .*

*Proof.* To compute the block degree of  $\zeta^{\mathbf{m}}(n_1, \dots, n_k)$ , we compute the block degree of

$$e_0 e_1 e_0^{n_1-1} e_1 e_0^{n_2-1} \dots e_1 e_0^{n_k-1} e_1$$

Now, if  $n_i > 1$ ,  $e_1 e_0^{n_i-1}$  contributes exactly  $n_i - 2$  repetitions, and hence contributes  $n_i - 2$  to the block degree. If  $n_i = 1$ , then we obtain an  $e_1^2$ , contributing  $1 = |1 - 2|$  to the block degree.  $\square$

**Remark 3.52.** Note that this gives us a relation among the weight, depth and block filtrations. To be precise, when restricted to  $\langle \zeta^{\mathfrak{m}}(n_1, \dots, n_k) : k \geq 1, n_i \geq 2 \rangle_{\mathbb{Q}}$ , we find  $\deg_{\mathcal{B}}(\zeta^{\mathfrak{m}}(n_1, \dots, n_k)) = n_1 + \dots + n_k - 2k$ , i.e block degree is weight minus twice depth. This is a special case of a more general relation

$$\deg_{\mathcal{B}}(\mathbb{I}^{\mathfrak{m}}(0; a_1, \dots, a_n; 1)) + 2d(\mathbb{I}^{\mathfrak{m}}(0; a_1, \dots, a_n; 1)) = n + 2\deg_{\mathcal{O}}(\mathbb{I}^{\mathfrak{m}}(0; a_1, \dots, a_n; 1))$$

where  $\deg_{\mathcal{O}}$  counts the number of occurrences of  $e_1^2$ .

We can see that, in terms of MZVs, block degree is naturally opposed to depth. As such, we can obtain the following formulation of the stuffle equations.

**Proposition 3.53.** *Let  $(m_1, \dots, m_k), (n_1, \dots, n_l)$  be two sequences of integers with  $m_i, n_j > 1$ ,  $k < l$ , and define  $m_{k+1} = \dots = m_l = 0$ . Then*

$$\sum_{\sigma \in Sh_{(l,k)}} \zeta^{\mathfrak{b}}(n_1 + m_{\sigma(1)}, \dots, n_l + m_{\sigma(l)}) = 0$$

*modulo products.*

*Proof.* This is precisely the lowest depth part of the stuffle equation modulo products. We claim this is the highest block degree part of the stuffle equation: In the stuffle equation, we obtain terms  $\zeta^{\mathfrak{m}}(s_1, \dots, s_t)$  where each  $s_r \in \{m_1, \dots, m_k, n_1, \dots, n_l\} \cup \{m_i + n_j | 1 \leq i \leq j\}$ . From our assumption on the values of  $m_i, n_j$ , this has block degree  $\sum_{i=1}^k m_i + \sum_{j=1}^l n_j - 2t$ . Maximising block degree is therefore equivalent to minimising  $t$ , so that all  $s_r \in \{n_1, \dots, n_l\} \cup \{m_i + n_j | 1 \leq i \leq j\}$ , which are precisely the terms obtained in the above sum.  $\square$

**Remark 3.54.** We can, in fact, extend Proposition 3.53 to allow  $m_i, n_j$  to be equal to 1, in light of Remark 3.52, by restricting the sum to include only terms that minimise  $\#\{i : m_i = 1\} + \#\{i : n_i = 1\} - k - l$  in the original stuffle equations.

As mentioned previously, the stuffle equations do not naturally see a description in terms of  $\mathfrak{bg}$ . However, we may, by a simple induction argument show the following weaker formulation

**Lemma 3.55.** *For any interval  $I = \{k, k+1, \dots, k+l\} \subset \{1, \dots, n\}$  of cardinality at least 2, and any  $f(x_1, \dots, x_n) \in \mathfrak{bg}$ , we have*

$$f(z_1, \dots, z_n) = 0$$

*where  $z_i = x_1$  if  $i \in I$ , and  $z_i = x_2$  otherwise*

*Proof.* Clearly, this holds for  $p_{2k+1}(x_1, x_2)$ . Thus, we may induct on block degree, and so it suffices to show that this holds for

$$f(x_1, x_2) \circ g(x_1, \dots, x_{n-1})$$

assuming it holds for  $g(x_1, \dots, x_{n-1}) \in \mathfrak{bg}$ . Suppose  $I = \{k, \dots, k+l\}$  is a fixed interval. Then, evaluating

$$\frac{1}{x_i} g(x_1, \dots, x_i, x_{i+2}, \dots, x_n) - \frac{1}{x_{i+1}} g(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$$

at  $(z_1, \dots, z_n)$  defined above, we obtain 0 by our induction hypothesis, except if  $I = \{k, k+1\}$ , and  $i \in \{k-1, k, k+1\}$ . If this is the case, we obtain three terms that are not immediately

zero by induction.

$$\begin{aligned} & \frac{f(x_1, x_2)}{x_1 - x_2} \left( \left( \frac{1}{x_1} - \frac{1}{x_2} \right) g(x_1, \dots, x_1, x_2, x_1, \dots, x_1) \right) \\ & + C \left( \left( \frac{1}{x_2} - \frac{1}{x_1} \right) g(x_1, \dots, x_1, x_2, x_1, \dots, x_1) \right) \\ & + \frac{f(x_2, x_1)}{x_2 - x_1} \left( \left( \frac{1}{x_2} - \frac{1}{x_1} \right) g(x_1, \dots, x_1, x_2, x_1, \dots, x_1) \right) \end{aligned}$$

which is clearly 0. Here,  $C = \lim_{x_1 \rightarrow x_2} \frac{f(x_1, x_2)}{x_1 - x_2}$ . Hence, the result holds for  $\{f, g\}$ , and thus for all elements of  $\mathfrak{bg}$ .  $\square$

We may hope to similarly define ‘block graded’ versions of the associator equations. While we can define a block filtration on the Lie algebra over which the pentagon equation is defined, it remains combinatorially challenging. The hexagon equation is not significantly simpler, but can to some extent be ignored, thanks to the following lemma.

**Lemma 3.56.** *Suppose  $\deg_{\mathcal{B}}(\mathcal{I}^{\mathfrak{m}}(0; a_1, \dots, a_n; 1)) > \lfloor \frac{n}{3} \rfloor$ . Then  $\mathcal{I}^{\mathfrak{b}}(0; a_1, \dots, a_n; 1) = 0$*

*Proof.* The Hoffman elements,  $\zeta^{\mathfrak{m}}(n_1, \dots, n_k)$ ,  $n_i \in \{2, 3\}$  span  $\mathcal{H}$ , and have

$$\deg_{\mathcal{B}}(\zeta^{\mathfrak{m}}(n_1, \dots, n_k)) = \#\{n_i : n_i = 3\}$$

Thus, every element of  $\mathcal{H}$  of weight  $n$  can be written as a linear combination of Hoffman elements of maximal block degree  $\lfloor \frac{n}{3} \rfloor$ . The result follows.  $\square$

**Proposition 3.57.** *The linearised hexagon equation*

$$\phi(e_0, e_1) + \phi(e_1, -e_0 - e_1) + \phi(-e_0 - e_1, e_0) = 0$$

*implies no non-trivial relations in  $gr^{\mathcal{B}}\mathcal{H}$ .*

*Proof.* Fix a word  $w$  and consider the coefficient of  $w$  in the hexagon equation. We obtain the following contributions

From  $\phi(e_0, e_1)$ , we obtain  $\mathcal{I}^{\mathfrak{m}}(0; w; 1)$ . From  $\phi(e_1, -e_0 - e_1)$ , we obtain  $\mathcal{I}^{\mathfrak{m}}(0; u; 1)$  where  $u$  has  $e_0$  only where  $w$  has  $e_1$ . From  $\phi(-e_0 - e_1, e_0)$ , we obtain  $\mathcal{I}^{\mathfrak{m}}(0; v; 1)$  where  $v$  has  $e_1$  only where  $w$  has  $e_0$ .

Considering terms of highest block degree of this form, we see that the block graded equation for a word of weight  $n$  involves only terms of the forms

$$\begin{aligned} & e_0^k e_1^{n-k} \\ & e_0^i e_1^j e_0^{n-i-j} \\ & e_1^i e_0^j e_1^{n-i-j} \end{aligned}$$

all of which have block degree at least  $n - 2$ , which is strictly greater than  $\lfloor \frac{n}{3} \rfloor$  for all  $n > 3$ . Thus, by Lemma 3.56, the only block graded equation of interest is in weight 3. Direct calculation shows the weight 3 equation to be an immediate consequence of duality  $\square$

### 3.11 The Ihara action in noncommuting variables

Using the isomorphism (3.3), we can define a vector space isomorphism

$$\mathbb{Q}\langle e_0, e_1 \rangle \xrightarrow{\sim} \mathbb{Q}\langle z_1, z_2, z_3, \dots \rangle =: \mathbb{Q}\langle Z \rangle$$

and hence an injection

$$\mathfrak{bg} \hookrightarrow \mathbb{Q}\langle Z \rangle$$

It can be helpful to consider functional equations satisfied by elements of  $\mathbf{bg}$  as properties of their images in  $\mathbb{Q}\langle Z \rangle$ . For example, the block shuffle relation corresponds to elements of  $\mathbf{bg}$  being primitive with respect to the coproduct defined by

$$\Delta z_n := z_n \otimes 1 + 1 \otimes z_n$$

Concatenation in  $\mathbb{Q}\langle Z \rangle$  corresponds to the polynomial multiplication given by

$$f(x_1, \dots, x_m) \cdots g(x_1, \dots, x_n) := f(x_1, \dots, x_m)g(x_{m+1}, \dots, x_{m+n})$$

We will use this to define the Ihara action in  $\mathbb{Q}\langle Z \rangle$ .

We need the following lemma.

**Lemma 3.58.** *The Ihara action is a derivation for this concatenation product.*

$$f \circ (g \cdot h) = (f \circ g) \cdot h + g \cdot (f \circ h)$$

*Proof.* Recall that, for  $f \in Q[x_1, \dots, x_m]$ ,  $F \in Q[x_1, \dots, x_n]$ , we define

$$(f \circ F)(x_1, \dots, x_{m+n-1}) = \sum_{i=1}^n \frac{f(x_i, \dots, x_{i+m-1})}{x_i - x_{i+m-1}} \left( \frac{F(x_1, \dots, x_i, x_{i+m}, \dots, x_{m+n-1})}{x_i} - \frac{F(x_1, \dots, x_{i-1}, x_{i+m-1}, \dots, x_{m+n-1})}{x_{i+m}} \right)$$

Hence, if  $F(x_1, \dots, x_n) = g(x_1, \dots, x_k)h(x_{k+1}, \dots, x_n)$ , we have

$$\begin{aligned} (f \circ g \cdot h) &= \sum_{i=1}^k \frac{f(x_i, \dots, x_{i+m-1})}{x_i - x_{i+m-1}} \left( \frac{g(x_1, \dots, x_i, x_{i+m}, \dots, x_{m+k-1})}{x_i} - \frac{g(x_1, \dots, x_{i-1}, x_{i+m-1}, \dots, x_{m+k-1})}{x_{i+m}} \right) h(x_{m+k}, \dots, x_{m+n-1}) \\ &\quad + \sum_{i=k+1}^n g(x_1, \dots, x_k) \frac{f(x_i, \dots, x_{i+m-1})}{x_i - x_{i+m-1}} \left( \frac{h(x_{k+1}, \dots, x_i, x_{i+m}, \dots, x_{m+n-1})}{x_i} - \frac{h(x_{k+1}, \dots, x_{i-1}, x_{i+m-1}, \dots, x_{m+n-1})}{x_{i+m}} \right) \end{aligned}$$

and so  $f \circ g \cdot h = (f \circ g) \cdot h + g \cdot (f \circ h)$ . □

Hence  $(f \circ -)$  is a derivation for concatenation in  $\mathbb{Q}\langle Z \rangle$ , and so, to define the Ihara action, it suffices to define  $f \circ z_n$ . We have

$$f \circ z_1^n = \frac{f(x_1, \dots, x_m)}{x_1 - x_m} (x_1^{n-1} - x_m^{n-1}) = f(x_1, \dots, x_n) \sum_{i+j=n-2} x_1^i x_m^j$$

Thus, we have that

$$f \circ z_n = \sum_{i+j=n-2} L_i R_j(f)$$

where  $L_i(z_n u) := z_{n+i} u$ , and  $R_j(u z_n) := u z_{n+j}$  are linear operators raising the first and last variables, respectively, in a word.

This also provides us with an alternative proof of Theorem 3.26, via the following equivalent statement.

**Proposition 3.59.** *The image of every  $\sigma \in \mathbf{bg}$  in  $\mathbb{Q}\langle Z \rangle$  is primitive with respect to the coproduct  $\Delta(z_n) = z_n \otimes 1 + 1 \otimes z_n$ .*

*Proof.* For this coproduct,  $\sigma$  primitive is equivalent to  $\sigma \in \text{Lie}[Z]$ . In block degree 1, we know this to be the case, as  $p_{2k+1}(x_1, x_2) + p_{2k+1}(x_2, x_1) = 0$ . It then suffices to show that, if  $\sigma, \psi \in \text{Lie}[Z]$ , that  $\sigma \circ \psi \in \text{Lie}[Z]$ . In particular, as we are interested in the image of  $\mathfrak{bg}$ , we may take  $\sigma$  to be in this image, and in fact, by associativity of the Ihara action, we may take  $\sigma$  to be of block degree 1. Finally, since the Ihara action is linear and a derivation, it suffices to show

$$([z_m, z_n]) \circ z_t \in \text{Lie}[Z]$$

This is easily verified.

$$\begin{aligned} ([z_m, z_n]) \circ z_t &= \sum_{i+j=t-2} L_i R_j [z_m, z_n] \\ &= \sum_{i+j=t-2} z_{m+i} z_{n+j} - z_{n+i} z_{m+j} \\ &= \sum_{i+j=t-2} z_{m+i} z_{n+j} - z_{n+j} z_{m+i} \\ &= \sum_{i+j=t-2} [z_{m+i}, z_{n+j}] \end{aligned}$$

Thus, for  $\sigma$  in the image of  $\mathfrak{bg}$ , and  $\psi \in \text{Lie}[Z]$ ,  $\sigma \circ \psi \in \text{Lie}[Z]$ , and we can therefore conclude that the image of  $\mathfrak{bg}$  is contained in  $\text{Lie}[Z]$ .  $\square$

## 4 Block relations and the double shuffle relations

While it remains unclear how to show that  $\mathfrak{bg}$  is indeed isomorphic to the algebra  $\mathfrak{bs}$  described in Remark 3.45, one approach is to show that the relations described imply the (block graded) double shuffle relationships. We claim this to be the case, and will show that, in block degree 1 and 2, the ‘block relations’ imply the block graded double shuffle relations.

We first show that the Hoffman regularisation relation is implied by the block relations. In particular, it suffices to show that

$$\sum_{\substack{0 \leq i \leq k-1 \\ n_{i+1} \neq 1}} \zeta^b(n_1, \dots, n_i, 1, n_{i+1}, \dots, n_k) \sum_{\substack{1 \leq i \leq k \\ n_i \neq 1}} \zeta^b(n_1, \dots, n_i + 1, \dots, n_k) = 0 \quad (4.1)$$

when each term is considered modulo products and  $n_k > 1$ .

**Lemma 4.1.** *The Hoffman regularisation relation holds for block graded multiple zeta values.*

*Proof.* Consider  $-I^{\text{bl}}(z_1 \sqcup z_{i_1} \dots z_{i_n}) = 0$ , with  $z_{i_1}, z_{i_n} > 1$ , so that  $z_{i_1} \dots z_{i_n}$  corresponds to a monomial in  $e_1 \mathbb{Q}\langle e_0, e_1 \rangle e_0$ . This is

$$-I^{\text{bl}}(z_1 z_{i_1} \dots z_{i_n}) - I^{\text{bl}}(z_{i_1} \dots z_{i_n} z_1) - \sum_{j=1}^{n-1} I^{\text{bl}}(z_{i_1} \dots z_{i_j} z_1 z_{i_{j+1}} \dots z_{i_n}) = 0$$

By shuffle regularisation

$$\begin{aligned} -I^{\text{bl}}(z_1 z_{i_1} \dots z_{i_n}) - I^{\text{bl}}(z_{i_1} \dots z_{i_n} z_1) &= I^{\text{bl}}(e_0 \sqcup w_1) - I^{\text{bl}}(z_1 z_{i_1} \dots z_{i_n}) + I^{\text{bl}}(e_1 \sqcup w_2) - I^{\text{bl}}(z_{i_1} \dots z_{i_n} z_1) \\ &= 2 \sum_{j=1}^n \sum_{2 < k < i_j} I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_k z_{i_j+1-k} \dots z_{i_n}) \\ &\quad + 3 \sum_{\substack{2 \leq j \leq n-1 \\ i_{j-1} \neq 1}} I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_1 z_{i_j} \dots z_{i_n}) \\ &\quad + \sum_{\substack{2 \leq j \leq n-1 \\ i_{j-1} = 1}} I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_1 z_{i_j} \dots z_{i_n}) \end{aligned}$$

Thus  $I^{\text{bl}}(z_1 \sqcup z_{i_1} \dots z_{i_n}) = 0$  is equivalent to

$$\sum_{j=1}^n \sum_{1 < k < i_j} I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_k z_{i_j+1-k} \dots z_{i_n}) + \sum_{\substack{2 \leq j \leq n-1 \\ i_{j-1} \neq 1}} I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_1 z_{i_j} \dots z_{i_n}) = 0$$

Now, if  $I^{\text{bl}}(z_{i_1} \dots z_{i_n})$  corresponds to  $(-1)^k \zeta^b(n_1, \dots, n_k)$ , then

$$\{I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_k z_{i_j+1-k} \dots z_{i_n})\}_{\substack{1 \leq j \leq n \\ 1 < j < i_j}}$$

corresponds bijectively to

$$\{(-1)^{k+1} \zeta^b(n_1, \dots, n_{j-1}, 1, n_j, \dots, n_k)\}_{n_j \neq 1 \neq n_{j+1}} \cup \{(-1)^k \zeta^b(n_1, \dots, n_j + 1, \dots, n_k)\}_{n_j \neq 2}$$

, and

$$\{I^{\text{bl}}(z_{i_1} \dots z_{i_{j-1}} z_k z_{i_j+1-k} \dots z_{i_n})\}_{\substack{1 < j < n \\ i_{j-1} \neq 1}}$$

corresponds bijectively to

$$\{(-1)^k \zeta^b(n_1, \dots, n_j, 1, n_{j+1}, \dots, n_k)\}_{n_j=1 \neq n_{j+1}} \cup \{(-1)^k \zeta^b(n_1, \dots, n_j + 1, \dots, n_k)\}_{n_j > 2}$$

and thus,  $I^{\text{bl}}(z_1 \sqcup z_{i_1} \dots z_{i_n}) = 0$  is equivalent to equation (4.1).  $\square$

We now turn to the double shuffle relations in block degree 1. The shuffle relations tell us that  $\mathbf{I}^{\mathbf{m}}(0; u \sqcup v; 1) = 0$  for all  $u, v \in \mathbb{Q}\langle e_0, e_1 \rangle$ . As we have considered the case where  $u = e_0$ , we can assume that  $u$  contains a  $e_0 e_1$  or an  $e_1 e_0$ , and that  $v$  a word of length at least 2, containing both  $e_0, e_1$ .

Thus in  $e_0(u \sqcup v)e_1$ , we can find a word containing both an  $e_1^2$  and an  $e_0^2$  that were not in  $v$ , and so  $\deg_{\mathcal{B}}(u \sqcup v) \geq \deg_{\mathcal{B}}(v) + 2$ , and hence there are no interesting shuffle relations in block degree 1.

Considering stuffle relations, we similarly see that a block degree 1 relation must arrive from  $\zeta^{\mathbf{m}}(u \star v)$  where  $\deg_{\mathcal{B}}(u) = 0$ ,  $\deg_{\mathcal{B}}(v) = 1$ , and so  $u = y_2^n$ , and  $v = y_2^a y_k y_2^b$  or  $v = y_3$ , where  $k \in \{1, 3\}$ . However, as there exists a term in the stuffle containing a  $y_4$  or a  $y_5$ , we obtain a term with block degree strictly greater than 1. Hence, there exist no nontrivial stuffle relations in block degree 1, and so the block relations imply the block graded double shuffle relations in block degree 1.

Similar analysis in block degree 2 shows that we need only to consider relations arising from  $\mathbf{I}^{\mathbf{m}}(e_1 e_0 \sqcup (e_1 e_0)^n) = 0$ , and  $\zeta^{\mathbf{m}}(y_2 \star y_2^n) = 0$  modulo products. We will consider first the stuffle relation.

Taking the block graded piece, we obtain that

$$\sum_{i=1}^n \zeta^{\mathbf{m}}(\{2\}^{i-1}, 4, \{2\}^{n-i}) = 0$$

which is equivalent to

$$\sum_{i=1}^n \mathbf{I}^{\mathbf{bl}}(z_{2i+1} z_1 z_{2n-2i+2}) = 0$$

which follows from the statement that, for all  $f(x_1, x_2, x_3) \in \mathbf{bg}$ ,  $\frac{\partial f}{\partial x_2}(x_1, 0, x_1) = 0$ . We know that  $f(x_1, x_2, x_3) = x_1 x_2 x_3 (x_1 - x_3) r(x_1, x_2, x_3)$ , and hence

$$\frac{\partial f}{\partial x_2}(x_1, 0, x_3) = x_1 x_3 (x_1 - x_3) r(x_1, 0, x_3)$$

from which the claim obviously follows.

Now, considering  $\mathbf{I}^{\mathbf{m}}(e_1 e_0 \sqcup (e_1 e_0)^n)$ , and taking the block degree 2 piece, we obtain that

$$\sum_{i=0}^{n-1} \sum_{j=0}^{n-i-1} \mathbf{I}^{\mathbf{bl}}((e_1 e_0)^i e_1^2 (e_0 e_1)^j e_0^2 (e_1 e_0)^{n-i-j-1}) = 0$$

or, equivalently

$$\sum_{i=0}^n \sum_{j=0}^{n-i-1} \mathbf{I}^{\mathbf{bl}}(z_{2i+2} z_{2j+2} z_{2n-2i-2j}) = 0$$

which we can rewrite once more as

$$\sum_{\substack{i+j+k=n+2 \\ i,j,k>0}} \mathbf{I}^{\mathbf{bl}}(z_{2i} z_{2j} z_{2k}) = 0$$

which follows from the statement that, for all  $f(x_1, x_2, x_3) \in \mathbf{bg}$ ,  $f_{eee}(x, x, x) = 0$ , where

$$f_{eee} := f(x_1, x_2, x_3) + f(-x_1, x_2, x_3) + f(x_1, -x_2, x_3) + f(-x_1, -x_2, -x_3)$$

Now, as  $f(x_1, x_2, x_3) = x_1 x_2 x_3 (x_1 - x_3) r(x_1, x_2, x_3)$ , for  $r \in \mathbf{rbg}$ , we have that

$$\begin{aligned} f(x, x, x) &= 0 \\ f(-x, x, x) &= 2x^4 r(-x, x, x) \\ f(x, -x, x) &= 0 \\ f(-x, -x, x) &= -2x^4 r(-x, -x, x) \end{aligned}$$

Additionally, the dihedral symmetry of  $\mathbf{rbg}$  implies that  $r(x, y, y) = r(x, x, y) = 0$ , and thus  $f_{eee} = 0$ .

Denote by  $\mathbf{bs}_n$  the block degree  $n$  piece of  $\mathbf{bs}$ . Define  $\mathbf{bsh}_n$  to be the vector subspace of  $\mathbf{dmr}_0$ , considered as a subspace of  $\mathbb{Q}\langle e_0, e_1 \rangle$ , satisfying the block degree  $n$  graded double shuffle relations. We have shown the following.

**Proposition 4.2.** *For  $n = 1, 2$ , we have inclusions of bigraded vector spaces*

$$\begin{array}{ccc} \mathbf{bg}_n & \hookrightarrow & \mathrm{gr}_{\mathcal{B}}^n \mathbf{dmr}_0 \\ \downarrow & & \downarrow \\ \mathbf{bs}_n & \hookrightarrow & \mathbf{bsh}_n \end{array}$$

## 5 An ungraded block shuffle

We wish to extend relations among block graded multiple zeta values to motivic multiple zeta values, modulo products. The work of Charlton [10] suggests that cyclic insertion holds at the level of motivic multiple zeta values. We shall introduce an extension of the block shuffle relation to motivic multiple zeta values, defined in work due to Hirose and Sato [23].

On algebra  $\mathbb{Q}\langle Z \rangle = \mathbb{Q}\langle z_1, z_2, \dots \rangle$ , define a quasi-shuffle product by linearly extending the following definition.

$$\begin{aligned} z_m u \hat{\sqcup} z_n v &:= z_m(u \hat{\sqcup} z_n v) + z_n(z_m u \hat{\sqcup} v) - L_{m+n}(u \hat{\sqcup} v) \\ u \hat{\sqcup} 1 &:= 1 \hat{\sqcup} u := u \end{aligned}$$

where

$$\begin{aligned} L_i(z_j u) &:= z_{i+j} u \\ L_i(1) &:= 0 \end{aligned}$$

Hirose and Sato show the following.

**Proposition 5.1.** *Let  $u, v \in \mathbb{Q}\langle Z \rangle$  be such that  $(u, v) \neq (z_1^m, z_1^a z_2^b z_1^b)$  or  $(z_1^a z_2^b z_1^b, z_1^m)$  for any  $m > 0, a, b \geq 0$ . Then*

$$I^m(u \hat{\sqcup} v) = 0$$

*considered modulo products.*

We can translate this into a statement about primitivity of elements of  $\mathfrak{g}^m$  with respect to the following coproduct, which we can readily check to be dual to the above quasi-shuffle product.

**Definition 5.2.** Define a coproduct on  $\mathbb{Q}\langle Z \rangle$  by

$$\begin{aligned} \Delta_{\text{bt}}(1) &:= 1 \otimes 1 \\ \Delta_{\text{bt}}(z_n) &:= \sum_{k \geq 0} (-1)^k \sum_{\substack{i_1 + \dots + i_{2k+1} = n \\ i_j > 0}} z_{i_1} \dots z_{i_k} \otimes z_{i_{k+1}} \dots z_{i_{2k+1}} + z_{i_{k+1}} \dots z_{i_{2k+1}} \otimes z_{i_1} \dots z_{i_k} \end{aligned} \quad (5.1)$$

Coassociativity of this coproduct is clear, and so we conclude the following.

**Lemma 5.3.** *This quasi-shuffle product is associative.*

We can equivalently reformulate Proposition 5.1 as the following statement.

**Proposition 5.4.** *For  $n > 0$ , define the vector space  $V_n := \mathbb{Q}z_1^n \oplus \bigoplus_{a+b=n-2} \mathbb{Q}z_1^a z_2^b z_1^b$ . Let  $\sigma \in \mathfrak{g}^m \subset \mathbb{Q}\langle Z \rangle$  be an element of weight  $N - 2$ . Then*

$$\Delta_{\text{bt}}(\sigma) - \sigma \otimes 1 - 1 \otimes \sigma \in \sum_{i+j=N} V_i \otimes V_j$$

While, discussing Hirose and Sato's argument is beyond the scope of this thesis, we can prove the following special case of Proposition 5.1.

**Proposition 5.5.** *For all  $i_1, \dots, i_n$  with  $i_1, i_n > 1$ .  $I^m(z_1 \hat{\sqcup} z_{i_1} \dots z_{i_n}) = 0$ .*

*Proof.* We claim this is a consequence of Hoffman's regularisation relation. In showing this, we will introduce the following abuse of notation.

$$\begin{aligned} I^m(e_{i_1} e_{i_2} \dots e_{i_n}) &:= I^m(0; i_1, i_2, \dots, i_n; 1) \\ I^m(n_1, \dots, n_k) &:= (-1)^k \zeta^m(n_1, \dots, n_k) \end{aligned}$$

Now, let  $w = e_1 e_{j_2} \dots e_{j_{N-1}} e_0$  be a monomial in  $\{e_0, e_1\}$ , let  $y_{n_1} \dots y_{n_k}$  be the image in the  $y$ -alphabet, and let  $z_{i_1} \dots z_{i_n}$  be the image of  $e_0 w e_1$  in the  $z$ -alphabet. Hoffman's regularisation relation tells us that

$$\mathbf{I}^{\mathbf{m}}(e_1 \sqcup w) - \mathbf{I}^{\mathbf{m}}(w e_1) = \sum_{i=0}^{k-1} \mathbf{I}^{\mathbf{m}}(n_1, \dots, n_i, 1, n_{i+1}, \dots, n_k) - \sum_{i=1}^k \mathbf{I}^{\mathbf{m}}(n_1, \dots, n_i + 1, \dots, n_k)$$

Via the duality relation, the left hand side is equal to

$$(-1)^{N+1} (\mathbf{I}^{\mathbf{m}}(e_0 \sqcup D w) - \mathbf{I}^{\mathbf{m}}(e_0 D w)) = (-1)^N \mathbf{I}^{\mathbf{m}}(z_1 z_{i_n} \dots z_{i_1})$$

The sum  $\sum_{i=0}^{k-1} \mathbf{I}^{\mathbf{m}}(n_1, \dots, n_i, 1, n_{i+1}, \dots, n_k)$  is equal to

$$\frac{1}{2} \left( \mathbf{I}^{\mathbf{m}}(e_1 \sqcup w) - \mathbf{I}^{\mathbf{m}}(w e_1) + I_{e_1^2} - I_{e_0^2} \right) = \frac{1}{2} \left( (-1)^N \mathbf{I}^{\mathbf{m}}(z_1 z_{i_n} \dots z_{i_1}) + I_{e_1^2} - I_{e_0^2} \right)$$

where  $I_{e_i^2} := \sum_{\substack{1 \leq k \leq N-1 \\ j_k = j_{k+1} = i}} \mathbf{I}^{\mathbf{m}}(e_1 \dots e_{j_k} e_1 e_{j_{k+1}} \dots e_0)$ . By considering when  $e_{j_k} = e_{j_{k+1}} = 1$  can occur, we see that

$$I_{e_1^2} = \sum_{\substack{1 < k \leq n \\ i_1 + \dots + i_k \equiv k+1 \pmod{2}}} \mathbf{I}^{\mathbf{m}}(z_{i_1} \dots z_{i_k} z_1 \dots z_{i_n})$$

and similarly

$$I_{e_0^2} = \sum_{\substack{1 < k \leq n \\ i_1 + \dots + i_k \equiv k \pmod{2}}} \mathbf{I}^{\mathbf{m}}(z_{i_1} \dots z_{i_{k-1}} z_{i_k + i_{k+1} + 1} z_{i_{k+2}} \dots z_{i_n})$$

Hence this first sum is equal to

$$\begin{aligned} & \frac{(-1)^N}{2} \left( \mathbf{I}^{\mathbf{m}}(z_1 z_{i_n} \dots z_{i_1}) \right. \\ & + \sum_{\substack{1 < k \leq n \\ i_1 + \dots + i_k \equiv k+1 \pmod{2}}} \mathbf{I}^{\mathbf{m}}(z_{i_1} \dots z_{i_k} z_1 \dots z_{i_n}) \\ & \left. - \sum_{\substack{1 < k \leq n \\ i_1 + \dots + i_k \equiv k \pmod{2}}} \mathbf{I}^{\mathbf{m}}(z_{i_1} \dots z_{i_{k-1}} z_{i_k + i_{k+1} + 1} z_{i_{k+2}} \dots z_{i_n}) \right) \end{aligned}$$

Next, consider the sum  $\sum_{i=1}^k \mathbf{I}^{\mathbf{m}}(n_1, \dots, n_i + 1, \dots, n_k)$ . We can similarly show that this is equal to

$$\begin{aligned} & \frac{(-1)^N}{2} \left( \mathbf{I}^{\mathbf{m}}(z_{i_n} \dots z_{i_1} z_1) \right. \\ & + \sum_{\substack{1 < k \leq n \\ i_1 + \dots + i_k \equiv k \pmod{2}}} \mathbf{I}^{\mathbf{m}}(z_{i_1} \dots z_{i_k} z_1 \dots z_{i_n}) \\ & \left. - \sum_{\substack{1 < k \leq n \\ i_1 + \dots + i_k \equiv k+1 \pmod{2}}} \mathbf{I}^{\mathbf{m}}(z_{i_1} \dots z_{i_{k-1}} z_{i_k + i_{k+1} + 1} z_{i_{k+2}} \dots z_{i_n}) \right) \end{aligned}$$

Combining these three equalities, and dividing through by  $\frac{(-1)^N}{2}$ , we obtain

$$\sum_{k=0}^n \mathbf{I}^{\mathbf{m}}(z_{i_n} \dots z_{i_{k+1}} z_1 z_{i_k} \dots z_{i_1}) - \sum_{k=1}^{n-1} \mathbf{I}^{\mathbf{m}}(z_{i_n} \dots, z_{i_{k+2}} z_{i_k + i_{k+1} + 1} z_{i_{k+2}} \dots z_{i_1}) = 0$$

which is precisely that  $\mathbf{I}^{\mathbf{m}}(z_1 \hat{\sqcup} z_{i_n} \dots z_{i_1}) = 0$ . □

**Remark 5.6.** As in Lemma 4.1, when we consider these motivic iterated integrals modulo products, this proof can be extended, identically, to obtain that  $I^m(z_1 \hat{\sqcup} z_{i_1} \dots z_{i_n}) = 0$  modulo products, for all  $z_{i_1} \dots z_{i_n} \notin \{z_1^{n-1} z_2, z_2 z_1^{n-1}\}$ . Associativity of this quasi-shuffle product then suggests Conjecture 5.1 could be strengthened to assume  $I^m(u \hat{\sqcup} v) = 0$  modulo products for all  $\{u, v\} \not\subset \{z_1^m, z_1^n z_2, z_2 z_1^n\}$ .

We make the following conjecture, based on numerical evidence, to somehow ‘block regularise’  $\mathfrak{g}^m$ .

**Conjecture 5.7.** Given  $\sigma \in \mathbb{Q}\langle Z \rangle$  of weight  $n$ , define  $\sigma^* := \frac{-c_\sigma}{n} (z_1^n z_2 - z_2 z_1^n)$ , where  $c_\sigma$  is the coefficient of  $z_1 z_{n+1}$  in  $\sigma$ . Then, for all  $\sigma \in \mathfrak{g}^m$ ,  $\sigma + \sigma^*$  is primitive with respect to  $\Delta_{\text{bf}}$ .

This regularisation is well defined.

**Lemma 5.8.** For any  $\sigma, \psi \in \mathfrak{g}^m$

$$\{\sigma + \sigma^*, \psi + \psi^*\} = \{\sigma, \psi\} + \{\sigma, \psi\}^*$$

*Proof.* The statement is equivalent to showing

$$\{\sigma, \psi\}^* = \{\sigma, \psi^*\} + \{\sigma^*, \psi\} + \{\sigma^*, \psi^*\}$$

As, for any element of  $\mathfrak{g}^m$  of Lie degree at least 2, all monomials have block degree at least 2 and hence  $c_\sigma = 0$ , it suffices to show that

1.  $\{\sigma, z_1^n z_2 - z_2 z_1^n\} = 0$  for all  $\sigma$  and any  $n$ .
2.  $\{z_1^m z_2 - z_2 z_1^m, z_1^n z_2 - z_2 z_1^n\} = 0$  for any  $m, n$ .

We begin by showing (2). Using that the Ihara action is a derivation, and noting that  $\sigma \circ z_1 = 0$  and  $\sigma \circ z_2 = \sigma$ , we see that

$$(z_1^m z_2 - z_2 z_1^m) \circ (z_1^n z_2 - z_2 z_1^n) = z_1^{m+n} z_2 - z_1^m z_2 z_1^n - z_1^n z_2 z_1^m + z_2 z_1^{m+n}$$

This expression is symmetric in  $m$  and  $n$ , and hence  $\{z_1^m z_2 - z_2 z_1^m, z_1^n z_2 - z_2 z_1^n\} = 0$ .

To show (1), we first note the following.

$$\sigma \circ (z_1^n z_2 - z_2 z_1^n) = z_1^n \sigma - \sigma z_1^n$$

We can assume that  $\sigma$  is homogeneous of block degree  $m-1$  without loss of generality. Switching to the language of commutative polynomials, supposing  $\sigma$  is represented by a polynomial  $f(x_1, \dots, x_m)$ , we obtain:

$$\begin{aligned} (z_1^n z_2 - z_2 z_1^n) \circ \sigma &= \sum_{i=1}^m \frac{x_i \dots x_{n+i} (x_{n+i} - x_i)}{x_i - x_{n+i}} \left( \frac{1}{x_i} \hat{f}(x_{i+1}, \dots, x_{i+n}) - \frac{1}{x_{i+n}} \hat{f}(x_i, \dots, x_{i+n-1}) \right) \\ &= - \sum_{i=1}^m x_{i+1} \dots x_{n+i} \hat{f}(x_{i+1}, \dots, x_{i+n} - x_i \dots x_{i+n-1} \hat{f}(x_i, \dots, x_{i+n-1})) \\ &= x_1 \dots x_n f(x_{n+1}, \dots, x_{m+n}) - x_{m+1} \dots x_{m+n} f(x_1, \dots, x_m) \\ &\equiv z_1^n \sigma - \sigma z_1^n \end{aligned}$$

where we have defined  $\hat{f}(x_i, \dots, x_{i+n-1}) := f(x_1, \dots, x_{i-1}, x_{i+n}, \dots, x_{m+n})$ . The result then follows.  $\square$

**Remark 5.9.** Hirose and Sato show that the block shuffle relation holds for all words  $u, v$  with some regularisation. It is as yet unknown if this regularisation agrees with that of Conjecture 5.7.

## 5.1 The block shuffle algebra

Assuming Conjecture 5.7, or taking any regularisation procedure, we can use the block shuffle relation to gain further information about both  $\mathfrak{g}^m$ , and the Lie coalgebra of motivic multiple zeta values  $\mathcal{L}$ , as follows.

As  $\mathfrak{g}^m$ , or rather a regularised  $\mathfrak{g}^m$ , is primitive with respect to  $\Delta_{\text{bl}}$ , there exists a map  $\mathfrak{g}^m \rightarrow \mathcal{P}(Z)$ , to the set of primitive elements of  $\mathbb{Q}\langle Z \rangle$ . We will provide an explicit generating set for  $\text{Lie}[\mathcal{P}(Z)] = \mathcal{P}(Z)$ .

**Proposition 5.10.**  $w_n := \sum_{k \geq 0} \frac{1}{2k+1} \sum_{\substack{i_1 + \dots + i_{2k+1} = n \\ 0 < i_j}} z_{i_1} \dots z_{i_{2k+1}}$  is primitive.

*Proof.* We first write  $\Delta_{\text{bl}}(w_n) = \sum_{r, s \geq 0} w_{r,s}$ , where

$$w_{r,s} \in \text{Span}\{z_{i_1} \dots z_{i_r} \otimes z_{j_1} \dots z_{j_s} \mid i_k, j_l \geq 0\}$$

is the degree  $(r, s)$  component. As  $\Delta_{\text{bl}}$  is cocommutative, to show  $w_n$  is primitive, it suffices to show that  $w_{r,s} = 0$  for all  $0 < r \leq s$ .

Next we note that, for fixed  $n_1, \dots, n_r$ , the projection of  $w_{r,s}$  onto  $z_{n_1} \dots z_{n_r} \otimes \mathbb{Q}\langle Z \rangle$  is in the  $\mathbb{Q}$ -span of  $\sum_{i_1 + \dots + i_s = n - n_1 - \dots - n_r} z_{n_1} \dots z_{n_r} \otimes z_{i_1} \dots z_{i_s}$ , by the symmetry in the definitions of  $w_n$  and  $\Delta_{\text{bl}}(z_n)$ . Thus, it suffices to compute the coefficient of this term for arbitrary  $n_1, \dots, n_r$ .

Considering a composition  $C = (c_1, \dots, c_m)$  of  $r$ , a sequence  $e = \{e_i\} \in \{\pm 1\}^{|C|}$ , and a sequence of integers  $0 < j_1 < \dots < j_m \leq 2k+1$ , this specifies a term in  $\sum_{i_1 + \dots + i_{2k+1} = n} z_{i_1} \dots z_{i_{2k+1}}$  given by

$$\prod_{u=1}^{j_1-1} (z_{i_u} \otimes 1 + 1 \otimes z_{i_u}) \prod_{t=1}^m \sum_{p_1 + \dots + p_{2c_t+e_t} = j_t} (z_{p_1} \dots z_{p_{c_t}} \otimes z_{p_{c_t+1}} \dots z_{p_{2c_t+e_t}}) \prod_{s=u}^{j_{t+1}-1} (z_{i_s} \otimes 1 + 1 \otimes z_{i_s})$$

The sign of this term is uniquely determined by  $(C, e)$  to be  $(-1)^r \prod_{i=1}^m e_i$ , and, summing over all possible choices of  $j_1, \dots, j_m$ , we obtain that the coefficient of this term is given by  $(-1)^r \prod_{i=1}^m e_i \frac{1}{2k+1} \binom{2k+1}{m}$ . We have a contribution to  $w_{r,s}$  when  $2k+1 - m + r + \sum_{i=1}^m e_i = s$ , and thus, the coefficient of  $\sum_{i_1 + \dots + i_s = n - n_1 - \dots - n_r} z_{n_1} \dots z_{n_r} \otimes z_{i_1} \dots z_{i_s}$  in  $w_{r,s}$  is given by

$$\sum_{m=1}^r \sum_{C \text{ a composition of } r \text{ into } m \text{ parts}} \sum_{e \in \{\pm 1\}^m} (-1)^r \prod_{i=1}^m e_i \frac{1}{s + m - r - \sum_{i=1}^m e_i} \binom{s + m - r - \sum_{i=1}^m e_i}{m}$$

Note that if  $\sum_{i=1}^m e_i = m - q$ , then  $\prod_{i=1}^m e_i = (-1)^q$ , and so we can replace the sum over  $e \in \{\pm 1\}^m$  with a sum over  $q$ , and perform the sum over compositions to obtain that this sum is equal to

$$\sum_{m=1}^r \sum_{q=0}^m (-1)^{r+q} \frac{1}{s - r + q} \binom{s - r + q}{m} \binom{r + m - 1}{m - 1} \binom{m}{q}$$

We will evaluate the sum

$$Q_m := \sum_{q=0}^m (-1)^q \frac{1}{s - r + q} \binom{s - r + q}{m} \binom{m}{q}$$

Denote by  $[x^i]f(x)$  the coefficient of  $x^i$  in  $f(x)$ ,  $f$  a polynomial in  $x$ . Then we have

$$\begin{aligned} Q_m &= [x^m] \sum_{q=0}^m \frac{(-1)^q}{s - r + q} (x+1)^{s-r+q} \binom{m}{q} \\ &= [x^m] \int_{-1}^x (y+1)^{s-r-1} \sum_{q=0}^m (-1)^q (y+1)^q \binom{m}{q} dy \\ &= [x^m] \int_{-1}^x (y+1)^{s-r-1} (-y)^m dy \\ &= 0 \text{ as the term of minimal degree is } x^{m+1} \end{aligned}$$

Hence,  $w_{r,s} = 0$  for all  $0 < r \leq s$ , and thus  $w_n$  is primitive.  $\square$

We can then, with this choice of  $w_n$ , generate all primitive elements.

**Proposition 5.11.** *The Lie algebra of primitives in  $\mathbb{Q}\langle Z \rangle$  with respect to  $\Delta_{\text{bl}}$  is equal to  $\text{Lie}[w_1, \dots, w_n, \dots]$ .*

*Proof.* Note that it is sufficient to show that any primitive element is contained in this Lie algebra. Suppose  $\sigma \in \mathbb{Q}\langle Z \rangle$  is primitive and homogeneous in weight, and let  $n$  be the minimum integer such that  $\sigma \in \mathcal{B}^n \mathbb{Q}\langle Z \rangle$ . Denoting by  $\bar{\sigma}$  the projection into  $\mathcal{B}^n \mathbb{Q}\langle Z \rangle / \mathcal{B}^{n+1} \mathbb{Q}\langle Z \rangle$ , we have that  $\bar{\sigma}$  is primitive with respect to  $\Delta(z_n) = z_n \otimes 1 + 1 \otimes z_n$ , and hence  $\bar{\sigma} \in \text{Lie}[Z]$ . Denote by  $T\bar{\sigma}$  the image of  $\bar{\sigma}$  under the map

$$\begin{aligned} \text{Lie}[Z] &\rightarrow \text{Lie}[w_1, \dots, w_n, \dots] \\ z_n &\mapsto w_n \end{aligned}$$

Then  $\sigma - T\bar{\sigma}$  is of strictly higher block degree than  $\sigma$ . As block degree is bounded above by weight, we can iterate this process to obtain a finite sequence of elements  $\sigma_1, \dots, \sigma_m \in \text{Lie}[w_1, \dots, w_n, \dots]$  such that  $\sigma = \sum_{i=1}^m \sigma_i \in \text{Lie}[w_1, \dots, w_n, \dots]$ .  $\square$

**Remark 5.12.** The work of Hirose and Sato, along side Proposition 5.11, suggests the existence of an injection  $\mathfrak{g}^{\text{m}} \rightarrow \text{Lie}[w_1, \dots, w_n, \dots]$ . However the following diagram does not commute.

$$\begin{array}{ccc} \mathfrak{g}^{\text{m}} & \hookrightarrow & \text{Lie}[w_1, \dots, w_n, \dots] \\ \downarrow & & \uparrow z_n \mapsto w_n \\ \mathfrak{bg} & \hookrightarrow & \text{Lie}[z_1, \dots, z_n, \dots] \end{array}$$

If we could choose an automorphism of  $\text{Lie}[w_1, \dots, w_n, \dots]$  mapping  $\{w_n\}_{n \geq 1} \rightarrow \{w'_n\}_{n \geq 1}$  to another set of generators, such that the composition

$$\mathfrak{bg} \hookrightarrow \text{Lie}[z_1, \dots, z_n, \dots] \xrightarrow{z_n \mapsto w'_n} \text{Lie}[w'_1, \dots, w'_n, \dots]$$

maps  $\mathfrak{bg}$  to the image of  $\mathfrak{g}^{\text{m}}$ , we could use this to define canonical  $\sigma_{2k+1}$ .

Dualising this map, we will obtain an isomorphism between the shuffle algebra  $(\mathbb{Q}\langle Z \rangle, \sqcup)$ , and the block shuffle algebra  $(\mathbb{Q}\langle Z \rangle, \hat{\sqcup})$ , which can be used to produce relations in  $\mathcal{L}$ , analogously to Hoffman's work on quasishuffle algebras [26], [24]. While the block shuffle product does not precisely fit Hoffman's definition of a quasi-shuffle product, most of his results can be reproduced.

**Definition 5.13.** A composition  $I$  of  $n$  is a sequence of positive integers  $(i_1, \dots, i_l)$  such that  $i_1 + \dots + i_l = n$ . Given a composition  $I$  of  $n$  into  $l$  parts and a composition  $J$  of  $l$  into  $k$  parts, we define the product composition:

$$J \circ I := (i_1 + \dots + i_{j_1}, i_{j_1+1} + \dots + i_{j_1+j_2}, \dots, i_{j_1+\dots+j_{k-1}+1} + \dots + i_{j_1+\dots+j_k})$$

Denote by  $\mathcal{C}(n)$  the set of compositions of  $n$ .

We define an action of compositions on  $\mathbb{Q}\langle Z \rangle$  as follows. Define  $[z_{a_1} \dots z_{a_k}] := z_{a_1+\dots+a_k}$ , and given a composition  $I$  of  $n$ , define

$$I[z_{a_1} \dots z_{a_n}] := [z_{a_1} \dots z_{a_{i_1}}][z_{a_{i_1+1}} \dots z_{a_{i_1+i_2}}] \cdots [z_{a_{i_1+\dots+i_{l-1}+1}} \dots z_{a_n}]$$

and  $I[w] = 0$  for any words not of length  $n$ .

**Proposition 5.14.** *Let  $\text{Tanh} : \mathbb{Q}\langle Z \rangle \rightarrow \mathbb{Q}\langle Z \rangle$  be the linear map with  $\text{Tanh}(1) = 1$  and, for  $w$  a word of length  $n$*

$$\text{Tanh}(w) = \sum_{(i_1, \dots, i_l) \in \mathcal{C}(n)} c_{i_1} \dots c_{i_l}(i_1, \dots, i_l)[w]$$

*where  $c_j$  is the coefficient of  $x^j$  in the Taylor expansion of  $\tanh(x)$ . Then  $\text{Tanh}$  is an algebra isomorphism*

$$\text{Tanh} : (\mathbb{Q}\langle Z \rangle, \sqcup) \rightarrow (\mathbb{Q}\langle Z \rangle, \hat{\sqcup})$$

To prove this, we require the following two lemmas. The first is due to Hoffman [26].

**Lemma 5.15.** *Let  $f(z) = c_1 z + c_2 z^2 + \dots$  be a function analytic at 0, with  $c_1 \neq 0$ , and  $c_i \in \mathbb{Q}$  for all  $i$ . Let  $f^{-1}(z) = b_1 z + b_2 z^2 + \dots$  be its inverse. Then the map  $\Psi_f : \mathbb{Q}\langle Z \rangle \rightarrow \mathbb{Q}\langle Z \rangle$  given by*

$$\Psi_f(w) = \sum_{(i_1, \dots, i_l) \in \mathcal{C}(n)} c_{i_1} \dots c_{i_l}(i_1, \dots, i_l)[w]$$

*for words of length  $n$ , and extended linearly has inverse  $\Psi_f^{-1} = \Psi_{f^{-1}}$ .*

We use this lemma to establish  $\text{Tanh}$  as the inverse map of a homomorphism  $\text{Tanh}^{-1}$  given by the dual of the coalgebra homomorphism  $z_n \mapsto w_n$ , hence avoiding having to establish that  $\text{Tanh}$  is a homomorphism directly.

**Lemma 5.16.** *The dual of  $\Phi : (\mathbb{Q}\langle Z \rangle, \Delta) \rightarrow (\mathbb{Q}\langle Z \rangle, \Delta_{\text{bl}})$ ,  $\Phi(z_n) := w_n$  is given by  $\Psi_{\text{tanh}^{-1}}$ , and defines a homomorphism  $\text{Tanh}^{-1} : (\mathbb{Q}\langle Z \rangle, \hat{\sqcup}) \rightarrow (\mathbb{Q}\langle Z \rangle, \sqcup)$ .*

*Proof.* As a consequence of Proposition 5.10,  $\Phi$  is a coalgebra homomorphism, and hence its dual will define an algebra homomorphism. Hence, it is sufficient to show that  $\Phi^* = \Psi_{\text{tanh}^{-1}}$ . Note that here, we view  $\mathbb{Q}\langle Z \rangle$  as its own graded dual via the pairing

$$\langle u, v \rangle = \delta_{u,v}$$

for monomials  $u, v$ . Thus

$$\Phi^*(w) = \sum_v \langle \Phi^* w, v \rangle v$$

taking the sum over all words. We see that

$$\begin{aligned} \langle \Phi^* w, z_{a_1} \dots z_{a_l} \rangle &= \langle w, \Phi(z_{a_1} \dots z_{a_l}) \rangle \\ &= \langle w, \prod_{i=1}^l \sum_{1 \leq 2k_i+1 \leq a_i} \frac{1}{2k_i+1} \sum_{i_1+\dots+i_{2k_i+1}=a_i} z_{i_1} \dots z_{i_{2k_i+1}} \rangle \end{aligned}$$

which is non-zero if and only if there exists some composition  $I = (i_1, \dots, i_l)$  of  $n$  into odd parts such that  $I[w] = v$ . The inner product then evaluates to  $\prod_{j=1}^l \frac{1}{i_j}$ . Thus

$$\Phi^*(w) = \sum_{\substack{(i_1, \dots, i_l) \in \mathcal{C}(n) \\ i_j \text{ odd}}} \frac{1}{i_1 \dots i_l} (i_1, \dots, i_l)[w]$$

which is precisely  $\Psi_{\text{tanh}^{-1}}$ . The result then follows.  $\square$

As a corollary to Proposition 5.14, we obtain the following.

**Corollary 5.17.**  *$(\mathbb{Q}\langle Z \rangle, \hat{\sqcup})$  is the free polynomial algebra on the Lyndon words.*

*Proof.* Hoffman's proof of Theorem 2.6 [26] applies exactly, inducting on the length of a word.  $\square$

**Corollary 5.18.** *Recall we have a surjective linear map  $I^b : \mathbb{Q}\langle Z \rangle \rightarrow \mathcal{L}$ , mapping a word to its corresponding iterated integral. Denote by  $L(Z)$  the  $\mathbb{Q}$ -span of the set of Lyndon words in  $Z$ . Then  $\mathcal{L} = I^b(L(Z))$ .*

*Proof.* Every word in  $\mathbb{Q}\langle Z \rangle$  can be written as a  $\hat{\sqcup}$ -polynomial in the Lyndon words. Proposition 5.1 tells us that the image of any terms of degree greater than 1 in this polynomial is 0, and hence  $I^b(w)$  is the image of the linear part, i.e.  $I^b(w) \in I^b(L(Z))$ .  $\square$

## 5.2 Further quasi-shuffle relations

We will also briefly comment on a way of producing further relations, drawing heavily from the work of Hoffman and Ihara [24]. We first recall one of their results, specialised to the case of block shuffle. In all that follows,  $\lambda$  is a formal parameter, and we extend  $\Psi_f$  by  $\Psi_f(\lambda) = \lambda$ .

**Definition 5.19.** Define  $\diamond : \mathbb{Q}Z \otimes \mathbb{Q}Z \rightarrow \mathbb{Q}Z$  by  $z_m \diamond z_n := z_{m+n}$ . Then, for any  $f(z) = c_1 z + c_2 z^2 + \dots$ , define

$$f_\bullet(\lambda w) := \sum_{i=1}^{\infty} \lambda^i c_i w^{\bullet i}$$

for  $\bullet \in \{\sqcup, \hat{\sqcup}\}$  and  $w \in \mathbb{Q}\langle Z \rangle$ , or  $\bullet = \diamond$  and  $w \in \mathbb{Q}Z$ .

**Remark 5.20.** In a slight abuse of notation, we shall write  $\exp_\bullet(w)$  for  $1 + f_\bullet(w)$  where  $f(z) = e^z - 1$ ; and  $\log_\bullet(1+w)$  for  $f_\bullet(w)$ , where  $f(z) = \log(1+z)$ , and similarly for  $\tanh_\bullet^{-1}(1+w)$ . Note that

$$\log_\bullet(\exp_\bullet(\lambda w)) = \lambda w \text{ and } \exp_\bullet(\log_\bullet(1 + \lambda w)) = 1 + \lambda w$$

**Proposition 5.21** (Theorem 5.1 [24]). *For any  $f(z) = c_1 z + c_2 z^2 + \dots$  and  $z \in \mathbb{Q}Z[[\lambda]]$ ,*

$$\Psi_f \left( \frac{1}{1 - \lambda z} \right) = \frac{1}{1 - f_\diamond(\lambda z)}$$

We also need a lemma due to Hoffman and Ihara.

**Lemma 5.22.** *For  $z \in \mathbb{Q}Z[[\lambda]]$*

$$\exp_{\hat{\sqcup}}(\lambda z) = \tanh \left( \frac{1}{1 - \lambda z} \right)$$

*Proof.* Since  $\tanh : (\mathbb{Q}\langle Z \rangle, \sqcup) \rightarrow (\mathbb{Q}\langle Z \rangle, \hat{\sqcup})$  is an algebra isomorphism, we must have that  $\tanh \circ f_\sqcup = f_{\hat{\sqcup}} \circ \tanh$ . Thus, as  $\tanh|_{\mathbb{Q}Z} = id$ , we have

$$\exp_{\hat{\sqcup}}(\lambda z) = \exp_{\hat{\sqcup}}(\tanh(\lambda z)) = \tanh(\exp_{\sqcup}(\lambda z)) = \tanh \left( \frac{1}{1 - \lambda z} \right)$$

where we have used that

$$\exp_{\sqcup}(\lambda z) = \sum_{n=0}^{\infty} \lambda^n \frac{z^{\sqcup n}}{n!} = \sum_{n=0}^{\infty} \lambda^n \frac{n! z^n}{n!} = \sum_{n=0}^{\infty} \lambda^n z^n$$

$\square$

Thus we can show the following

**Proposition 5.23.** *For  $z \in \mathbb{Q}A[[\lambda]]$*

$$\exp_{\hat{\sqcup}}(\tanh_{\diamond}^{-1}(1 + \lambda z)) = \frac{1}{1 - \lambda z}$$

*Proof.* By Lemma 5.22, this is equivalent to showing that

$$\text{Tanh}\left(\frac{1}{1 - \tanh_{\diamond}^{-1}(1 + \lambda z)}\right) = \frac{1}{1 - \lambda z}$$

However, this follows immediately from the statement of Propostion 5.21 for  $f = \tanh^{-1}$ .  $\square$

**Corollary 5.24.** *For any  $z \in \mathbb{Q}Z$  and any  $n > 1$ ,  $I^b(z^n) = 0$ .*

*Proof.* Taking the image of the equality in Proposition 5.23, we obtain

$$I^b(1 + \tanh_{\diamond}^{-1}(1 + \lambda z) + \sum_{n \geq 2} \frac{\tanh_{\diamond}^{-1}(\lambda z)^{\hat{\cup} n}}{n!}) = \sum_{n \geq 0} \lambda^n I^b(z^n)$$

As  $I^b$  kills  $\hat{\cup}$ -products, the left hand side is just  $\lambda I^b(z)$ . Comparing coefficients of  $\lambda^n$ , we see that  $I^b(z^n) = 0$  for all  $n > 1$ .  $\square$

**Remark 5.25.** As  $I^b(w) = 0$  if the length of  $w$  and the weight of  $w$  are of the same parity, we see that we must have  $z \in \bigoplus_{i=1}^{\infty} \mathbb{Q}z_2 i$ , and  $n$  odd for the statement to be non-trivial.

**Example 5.26.** Consider  $z = z_2$ , then  $I^b(z_2^{2k+1})$  is the image of  $\zeta^a(\{1, 3\}^k)$  in  $\mathcal{L}$ , and thus  $\zeta^a(\{1, 3\}^k) = 0 \bmod \text{products}$ . It is known, due the work of Broadhurst [?] that we infact have  $\zeta(\{1, 3\}^k) = \frac{2\pi^{4k}}{4k+2}$ .

If we consider  $z = z_4$ , we see that  $\zeta^a(\{2, 1, 2, 3, 2\}^k) = 0 \bmod \text{products}$ . Similarly, taking  $z = z_2 + z_4$ , we obtain that  $\zeta^a(\{1, 2, 3\}^k) = 0 \bmod \text{products}$ .

## 6 Finite characteristic, p-adic, and integer solutions to the double shuffle equations

In our search for rational associators, we may wish to consider the existence of simpler solutions. For example, if we restrict to associators with integer coefficients, is it easier to find a solution? The double shuffle equations are defined over the integers, and so can be considered modulo primes. Can we find an  $\mathbb{F}_p$  solution, or a  $\mathbb{Q}_p$  solution? What about a solution in any field of positive characteristic  $p$ ?

The question of  $p$ -adic associators has been considered previously by Furusho, and Alekseev, Podkopaeva and Severa. In [20], Furusho defines  $p$ -adic analogues of multiple zeta values as elements of  $\mathbb{C}_p$ , showing the existence of a grouplike element of  $\mathbb{C}_p\langle\langle e_0, e_1 \rangle\rangle$ , before going on to show that these  $p$ -adic multiple zeta values are elements of  $\mathbb{Q}_p$ . Alekseev et. al. define a class of grouplike elements of  $\mathbb{Q}_p\langle\langle e_0, e_1 \rangle\rangle$ , that they call natural associators, satisfying certain upper bounds on their  $p$ -adic valuation [?].

Thus we will focus instead on  $\mathbb{F}_p$  solutions to the double shuffle equations. In fact, we can show that there are no non-trivial solutions to the shuffle equations with coefficients in  $\mathbb{F}_p$ . We begin by recalling the definition of a shuffle algebra over a field  $k$

**Definition 6.1.** Given an alphabet  $X = \{x_1, x_2, \dots, x_n\}$ , we define the shuffle algebra  $\text{Sh}(R)$  over a ring  $R$  to be the  $R$ -module  $R\langle X \rangle$  equipped with the shuffle product, which we define recursively for  $u, v$  words in  $X$ , by

$$\begin{aligned} u \sqcup 1 &= 1 \sqcup u = u \\ x_i u \sqcup x_j v &= x_i (u \sqcup x_j v) + x_j (x_i u \sqcup v) \end{aligned}$$

It is easy to check that this defines a commutative associative algebra structure on  $R\langle X \rangle$ .

In particular, if we consider  $k = \mathbb{F}_p$ ,  $p$  prime, we find the following decomposition.

**Proposition 6.2.** Let  $\phi_p : \text{Sh}(\mathbb{F}_p) \rightarrow \text{Sh}(\mathbb{F}_p)$  denote the ‘shuffle Frobenius’ map, sending  $u \mapsto u^{\sqcup p}$ , the shuffle product of  $p$  copies of  $u$ . Then  $\text{Sh}(\mathbb{F}_p) = \mathbb{F}_p \oplus \ker \phi_p$ .

*Proof.* First note that, for any commutative product  $\times$ , and any  $a, b \in \mathbb{F}_p\langle X \rangle$ ,  $(a + b)^{\times p} = a^{\times p} + b^{\times p}$ . Hence,  $\phi_p$  is linear, and so, as  $\phi_p|_{\mathbb{F}_p} = \text{id}_{\mathbb{F}_p}$ , it suffices to show that for a word  $u$  in  $X$ ,  $\phi_p(u) = 0$ .

Let  $u = x_i v$ . Then

$$\begin{aligned} \phi_p(u) &= x_i v \sqcup x_i v \sqcup \dots \sqcup x_i v \\ &= \sum_{k=1}^p x_i (x_i v \sqcup \dots \sqcup v \sqcup \dots \sqcup x_i v) \end{aligned}$$

where we take the  $x_i$  from the  $k^{\text{th}}$  copy of  $x_i v$ . But as the shuffle product is commutative, we find

$$\begin{aligned} \phi_p(u) &= \sum_{k=1}^p x_i (v \sqcup x_i v \sqcup \dots \sqcup x_i v) \\ &= p x_i (v \sqcup x_i v \sqcup \dots \sqcup x_i v) = 0 \end{aligned}$$

□

As grouplike elements of  $k\langle\langle e_0, e_1 \rangle\rangle$  define homomorphisms from the shuffle algebra to  $k$ , we can use this proposition to obtain information about grouplike elements of  $\mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$ .

**Theorem 6.3.** There are no non-trivial grouplike elements of  $\mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$ .

*Proof.* Suppose  $\Phi \in \mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$  is grouplike. Then  $\Phi$  we can consider  $\Phi$  as a homomorphism  $\text{Sh}(\mathbb{F}_p) \rightarrow \mathbb{F}_p$ , mapping a word  $u$  to the coefficient of  $u$  in  $\Phi = \sum_{w \in \{e_0, e_1\}^\times} c_w w$ .

As  $\Phi$  is a homomorphism, we have, for all  $w \neq 1$

$$\Phi(w) = \Phi(w)^p = \Phi(w^{\sqcup p}) = \Phi(0) = 0$$

where the final two equalities follow from Proposition 6.2. Hence  $\Phi = \sum_{w \in \{e_0, e_1\}^\times} \Phi(w)w = 1$ .  $\square$

**Remark 6.4.** Note that at no point in the proofs of Proposition 6.2, nor Theorem 6.3 do we use any properties of  $\mathbb{F}_p$  beyond having positive characteristic. Hence, both results hold over any field of positive characteristic.

**Corollary 6.5.** *There exist no non-trivial grouplike elements of  $\mathbb{Z}\langle\langle e_0, e_1 \rangle\rangle$ .*

*Proof.* Suppose  $\Phi = \sum_{w \in \{e_0, e_1\}^\times} c_w w \in \mathbb{Z}\langle\langle e_0, e_1 \rangle\rangle$  is grouplike. Fix a word  $u \neq 1$  in  $\{e_0, e_1\}$ , and define  $u_R^* : R\langle\langle e_0, e_1 \rangle\rangle \rightarrow R$  to be the  $R$ -linear map sending  $u$  to 1 and all other words to 0.

Then we have the following commutative diagram

$$\begin{array}{ccc} \mathbb{Z}\langle\langle e_0, e_1 \rangle\rangle & \xrightarrow{u_{\mathbb{Z}}^*} & \mathbb{Z} \\ \downarrow & & \downarrow \\ \mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle & \xrightarrow{u_{\mathbb{F}_p}^*} & \mathbb{F}_p \end{array}$$

and, as a consequence of Theorem (6.3),  $u_{\mathbb{F}_p}^*$  is the zero map, for all  $p$ . Hence, the composition

$$\mathbb{Z}\langle\langle e_0, e_1 \rangle\rangle \xrightarrow{u_{\mathbb{Z}}^*} \mathbb{Z} \longrightarrow \prod_{p \text{ prime}} \mathbb{F}_p$$

is the zero map. The second map is injective, and so  $u_{\mathbb{Z}}^*$  is the zero map for every  $u \neq 1$ . Thus  $\Phi = 1$ .  $\square$

Thus we can have no integer grouplike elements of  $\mathbb{Q}\langle\langle e_0, e_1 \rangle\rangle$ .

**Remark 6.6.** The proof of Corollary 6.5 is distinctly overkill. The result also follows if we let  $c_w$  be the coefficient of  $w$  in  $\Phi$ , and note that  $c_{w^{\sqcup n}} = \frac{c_w^n}{n!}$  for  $\Phi$  grouplike. As this tends to 0 as  $n$  grows, we cannot have every coefficient be integral.

**Remark 6.7.** As noted previously, Theorem 6.3 holds for any field of positive characteristic. In particular, if  $k$  is a number field, and  $\mathfrak{p}$  an ideal of  $\mathcal{O}_k$  then the result holds for series with coefficients in  $\mathcal{O}_k/\mathfrak{p}\mathcal{O}_k$ . We can then show the analogous corollary and conclude that there exist no non-trivial grouplike elements of  $\mathcal{O}_k\langle\langle e_0, e_1 \rangle\rangle$ .

We can extend Theorem 6.3 to say something about grouplike elements of  $\mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$ , showing that they cannot exist.

**Theorem 6.8.** *There does not exist a non-trivial grouplike element of  $\mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$ .*

*Proof.* Suppose  $\Phi \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$  is grouplike. We have a natural projection from  $\mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle \rightarrow \mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$ , and we will denote the image of any  $\Psi \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$  under this projection by  $\bar{\Psi}$ . As a consequence of Theorem 6.3, we see that we can write  $\Phi = 1 + p\Phi_1$ . Considering the projection modulo  $p^2$ , we find that

$$p\Delta\Phi_1 \equiv p\Phi_1 \otimes 1 + 1 \otimes p\Phi_1 \pmod{p^2}$$

and hence  $\bar{\Phi}_1$  is primitive. For any field  $k$ , the primitive elements of  $k\langle\langle e_0, e_1 \rangle\rangle$  are precisely elements of  $\hat{Lie}_k(e_0, e_1)$ , the degree completion of the free Lie algebra. Writing  $\bar{\Phi}_1$  in  $\mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$  as an element of  $\hat{Lie}_{\mathbb{F}_p}(e_0, e_1)$ , we consider the natural “inverse” to write

$$\Phi_1 = \Psi_1 + p\Phi_2$$

where  $\Psi_1 \in \hat{Lie}_{\mathbb{Z}_p}(e_0, e_1)$  is primitive and has coefficients in  $\{0, 1, \dots, p-1\}$ . Considering the projection of  $\Phi$  modulo  $p^3$ , we obtain that

$$\Delta\bar{\Phi}_2 = \bar{\Phi}_2 \otimes 1 + \bar{\Psi}_1 \otimes \bar{\Psi}_1 \otimes \bar{\Phi}_2$$

and so

$$\bar{\Phi}_2 = \frac{1}{2}\bar{\Psi}_1^2 + \text{a primitive element of } \mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$$

We can once again lift this to obtain that

$$\Phi = 1 + p\Psi_1 + p^2\Psi_2 + p^3\Phi_3$$

where  $\Delta\Psi_2 = \Psi_2 \otimes 1 + \Psi_1 \otimes \Psi_1 + 1 \otimes \Psi_2$ . We can repeat this process, considering  $\Phi$  modulo higher powers of  $p$  to obtain a series of elements  $\Psi_n$  such that

$$\begin{aligned} \Delta\Psi_n &= \Psi_n \otimes 1 + 1 \otimes \Psi_n + \sum_{i=1}^{n-1} \Psi_i \otimes \Psi_{n-i} \\ \Phi &= 1 + \sum_{i=1}^n p^i \Psi_i + p^{n+1} \Phi_{n+1} \end{aligned}$$

for some  $\Phi_{n+1} \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$ . These equations determine  $\Psi_n$  as a unique polynomial in  $\Psi_1, \dots, \Psi_{n-1}$ , up to addition of a primitive element. However, considering the projections in  $\mathbb{F}_p\langle\langle e_0, e_1 \rangle\rangle$ , we find that the coefficient of  $\bar{\Psi}_1^p$  in the polynomial determining  $\bar{\Psi}_p$  would be  $\pm \frac{1}{p}$ , and hence cannot be determined. Thus, given any  $\Psi_1, \dots, \Psi_{p-1} \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$ , we cannot find a  $\Psi_p \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$ . Thus, no nontrivial grouplike element of  $\mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$  exists.

To see that the coefficient of  $\bar{\Psi}_1^p$  should be  $\pm \frac{1}{p}$ , consider the following. Denote by  $c_a^{(k)}$  the coefficient of  $\bar{\Psi}_1^a \bar{\Psi}_k \bar{\Psi}_1^{p-k-2}$  in  $\bar{\Psi}_p = P(\bar{\Psi}_1, \dots, \bar{\Psi}_{p-1})$  for  $k \geq 2$ , and  $c^{(1)}$  the coefficient of  $\bar{\Psi}_1^p$ . In order to satisfy

$$\Delta\bar{\Psi}_p = \bar{\Psi}_p \otimes 1 + 1 \otimes \bar{\Psi}_p + \sum_{i=1}^{n-1} \bar{\Psi}_i \otimes \bar{\Psi}_{n-i}$$

we must have that the coefficient of  $\bar{\Psi}_1^{p-k} \otimes \bar{\Psi}_k$  is 0 in  $\Delta\bar{\Psi}_p$ .

We can obtain  $\bar{\Psi}_1^{p-k} \otimes \bar{\Psi}_k$  only in the coproduct of  $\bar{\Psi}_1^a \bar{\Psi}_{k+1} \bar{\Psi}_1^{p-k-a-1}$  and of  $\bar{\Psi}_1^a \bar{\Psi}_i \bar{\Psi}_1^{p-k-a}$  and hence we must have

$$\sum_{a=0}^{p-k} c_a^{(k)} + \sum_{a=0}^{p-k-1} c_a^{(k+1)} = 0$$

and hence

$$\sum_{a=0}^{p-2} c_a^{(2)} = \pm \left( c_0^{(p-1)} + c_1^{(p-1)} \right)$$

We can easily see that  $c_0^{(p-1)} + c_1^{(p-1)} = 1$ , and thus  $\sum_{a=0}^{p-2} c_a^{(2)} = \pm 1$ .

Finally, considering the coefficient of  $\bar{\Psi}_1^{p-1} \otimes \bar{\Psi}_1$ , we see that

$$pc^{(1)} = \sum_{a=0}^{p-2} c_a^{(2)} = \pm 1$$

which, as this equation holds in  $\mathbb{F}_p$ , gives an immediate contradiction.  $\square$

This provides an immediate answer to a question suggested by Furusho about the  $p$ -adic integrality of his  $p$ -adic multiple zeta values: the cannot all be elements of  $\mathbb{Z}_p$ , as they would otherwise define a counter example to the above theorem. Additionally, we cannot have a grouplike element  $\Phi = 1 + \sum_{w \in \{e_0, e_1\}^\times} c_w w$  of  $\mathbb{Q}_p\langle\langle e_0, e_1 \rangle\rangle$  for which the valuations of  $c_w$  are bounded below.

**Remark 6.9.** The contradiction occuring when calculating  $\Psi_p$  is reminiscent of Deligne's description of the motivic fundamental group of a smooth scheme [13]. In describing the  $\ell$ -adic realisation, he notes that the  $N$ -th quotient by the descending central series has a  $\mathbb{Z}_\ell$ -structure only for  $N < \ell$ , which has obvious parallels with the above result.

**Corollary 6.10.** Define  $\nu_p(\Phi)$ , for  $\Phi = 1 + \sum_{w \in \{e_0, e_1\}^\times} c_w w \in \mathbb{Q}_p\langle\langle e_0, e_1 \rangle\rangle$ , by

$$\nu_p(\Phi) := \inf\{\nu_p(c_w) : w \in \{e_0, e_1\}^\times\}$$

where  $\nu_p(c_w)$  is the normal  $p$ -adic valuation. Then, for any non-trivial grouplike  $\Phi$ ,  $\nu_p(\Phi) = -\infty$ .

*Proof.* Let  $\Phi$  be a grouplike element of  $\mathbb{Q}_p\langle\langle e_0, e_1 \rangle\rangle$ . If  $\nu_p(\Phi) \geq 0$ , then  $\Phi \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$ , then  $\Phi$  is trivial by Theorem 6.8. Otherwise, if  $\nu_p(\Phi) = -N$ , for some  $N > 0$ , consider the element  $\tilde{\Phi} \in \mathbb{Z}_p\langle\langle e_0, e_1 \rangle\rangle$  obtained as the image of  $\Phi$  under the mapping

$$e_i \mapsto p^N e_i$$

This is clearly  $p$ -adically integral, and, as this map is an automorphism of grouplike elements, must be trivial. The map is also invertible, and hence we must have  $\Phi = 1$ . Thus, any grouplike element with finite valuation is trivial.  $\square$

**Remark 6.11.** A consequence of this argument is that  $\nu_p(c_{uv}) \geq \nu_p(c_u) + \nu_p(c_v)$ . A similar argument, considering grouplike elements of  $\mathbb{C}[[t]]\langle\langle e_0, e_1 \rangle\rangle$ , show that any sufficiently 'nice' valuation is also superadditive. Weight and depth are examples of such valuations. Block degree is not, as an essential condition is a compatibility with the shuffle product.

**Corollary 6.12.** Let  $\Phi = 1 + \sum_{w \in \{e_0, e_1\}^\times} c_w w$  be grouplike with coefficients in  $\mathbb{Q}_p$  and let  $v$  be a word of weight  $n$ . Then, for all non-negative  $a, b$  such that  $3a + 2b = n$ ,  $\nu_p(c_v) \geq a\nu_p^{(3)} + b\nu_p^2$ , where

$$\nu_p^j := \min\{\nu_p(c_u) : u \text{ is of weight } j\}$$

*Proof.* As noted in Remark 6.11, the  $p$ -adic valuation is superadditive with respect to concatenation. Thus, for any factorisation  $v = v_1 \dots v_k$ , we have  $\nu_p(c_v) \geq \nu_p(c_{v_1}) + \dots + \nu_p(c_{v_k})$ . The result follows immediately  $\square$

We contrast this result with those of Alekseev, Podkopaeva and Severa [?], who show the following

**Theorem 6.13.** There exist associators with rational coefficients  $\phi \in 1 + \sum_{n \geq 1} p^{-b_p(n)} \mathbb{Z}_p\langle e_0, e_1 \rangle^n$  for all  $p$ , where  $R\langle e_0, e_1 \rangle$  is the space of  $R$ -linear combinations of weight  $n$  monomials, and

$$b_p(n) := \left( \frac{pn}{(p-1)^2} - \frac{1}{p-1} \right)$$

While this is at first glance an existence result rather than a global bound, they show as a corollary

**Corollary 6.14.** *For  $p > 2$  prime, let  $(\lambda, f) \in GT(\mathbb{Q}_p)$  be such that  $\lambda \in 1 + p\mathbb{Z}_p^*$  and*

$$f \in 1 + p\mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{\geq 1} + \mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{\geq p-1}$$

*Then  $\psi := \ln(f)/\ln(\lambda) \in \mathfrak{gt}(\mathbb{Q}_p)$  is of the form*

$$\psi \in \mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle + \sum_{s \geq 0} p^{-s-1} \mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{geqp^s(p-1)}$$

*where  $GT$  and  $\mathfrak{gt}$  are the (prounipotent) Grothendieck-Teichmuller group and Lie algebra, respectively, and  $\hat{e}_i := \exp(e_i) - 1$ .*

## 7 References

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