Rational structures on multiple zeta values

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Abstract

Motivated originally by the question of defining a rational canonical associator, we study rational structures associated to multiple zeta values. In particular, we focus on the question of providing an explicit description of the motivic Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ associated to $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ via new families of motivic relations among multiple zeta values.

Inspired by results obtained by considering depth-graded multiple zeta values, we attempt a similar approach. We introduce the block filtration on the space of multiple zeta values and show that it agrees with the coradical filtration induced by the motivic coaction. By considering the associated graded Lie algebra of $\mathfrak{g}^{\mathfrak{m}}$ with respect to this filtration, we obtain an isomorphic Lie algebra $\mathfrak{bg}$ with canonical representatives for its generators in $\mathbb{Q}\langle e_0, e_1\rangle$. This provides a possible route to defining canonical generators of $\mathfrak{g}^{\mathfrak{m}}$ by finding a section of the projection induced on $\mathbb{Q}\langle e_0, e_1\rangle$ by this isomorphism.

We then consider relations among block graded motivic multiple zeta values, finding several new families of relations and providing a complete description of $\mathfrak{bg}$ in low block degree. We use the motivic coaction to lift these relations to genuine relations among motivic multiple zeta values, providing new families of relations and generalising previously known relations such as those due to Borwen, Bradley, Broadhurst and Lisonek.

Finally, we consider the implication of previously known relations on the p-adic valuation of coefficients of a rational associator, providing a bound on the growth in terms of weight and block degree. We also present a partial solution to the question of canonical generators via the introduction of an inner product.

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Part I

The Block Filtration

Chapter 1

Background

1.1 Introduction

1.1.1 Goals

Multiple zeta values (MZVs) are a class of interesting transcendental numbers, going back to Euler in the 1700s and generalising values of the Riemann zeta function at integer argument. While they were not a focus of mathematical research for many years, there has been a recent resurgence of interest in these numbers. They have been found arising naturally in many areas of mathematics and physics: in generalisations of modular forms, in quantum field theory and high energy physics, in knot theory, in the study of the absolute Galois group of the rationals, in quantum algebra, and in the theory of associators. They also arise naturally as periods of mixed Tate motives [9].

The Tannakian category $\mathcal{MT}(\mathbb{Z})$ of mixed Tate motives over $\mathrm{Spec}(\mathbb{Z})$ is equivalent to the category of finite dimensional representations of an affine group scheme called its Galois group $\mathrm{G}_{\mathcal{MT}(\mathbb{Z})}$. It is well known [17] that this group decomposes as a semidirect product of the multiplicative group and a pro-unipotent group

$$\mathrm{G}_{\mathcal{MT}(\mathbb{Z})} \cong \mathbb{G}_m \ltimes U_{\mathcal{MT}(\mathbb{Z})}.$$

$U_{\mathcal{MT}(\mathbb{Z})}$ has graded Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ that is non-canonically isomorphic to a free Lie algebra with generators in odd weight

$$\mathfrak{g}^{\mathfrak{m}} \cong \mathrm{Lie}[\sigma_3, \sigma_5, \ldots]$$

called the motivic Lie algebra. This Lie algebra is related to several problems, having ties to the Grothendieck-Teichmuller group [38] and associators [19], and injecting into Racinet's double shuffle Lie algebra $\mathfrak{dmr}_0$ [38]. The connection to associators and the Grothendieck-Teichmuller group is particularly interesting, suggesting an explicit description of $\mathfrak{g}^{\mathfrak{m}}$ could be used to construct an explicit rational associator. This would be a powerful computational tool, allowing construction of universal knot invariants, quasi-triangular Hopf algebras, and solving problems in quantisation-deformation.

As MZVs arise as periods of mixed Tate motives, we obtain an action of $\mathrm{G}_{\mathcal{MT}(\mathbb{Z})}$ on (motivic) MZVs. In fact, the Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ is known to be dual to (motivic) MZVs, in the following sense: in [27], Goncharov defines a bialgebra $\mathcal{A}$ of unipotent de Rham multiple zeta values, formal analogues to multiple zeta values (modulo $\zeta(2)$), endowed with a coproduct. Brown [9] extends this definition to a comodule $\mathcal{H}$ over the graded ring of affine functions over $\mathrm{G}_{\mathcal{MT}(\mathbb{Z})}$, called motivic multiple zeta values. This algebra, along with its coaction

$$\Delta : \mathcal{H} \to \mathcal{A} \otimes \mathcal{H}$$

encodes all motivic relations among MZVs. We have that $\mathcal{A} = \mathcal{H}/(\zeta^{\mathfrak{m}}(2))$, where $\zeta^{\mathfrak{m}}(2)$ is the motivic analogue of $\zeta(2)$. Taking the Lie coalgebra of indecomposables of $\mathcal{A}$, we obtain the dual of $\mathfrak{g}^{\mathfrak{m}}$.

Remark 1.1.1. We take our convention as identifying $e_i \leftrightarrow \frac{dz}{z-i}$, so that elements of $\mathfrak{g}^{\mathfrak{m}}$ describe relations among iterated integrals, rather than multiple zeta values. As such, our results are 'depth-signed'.

Providing an explicit injection $\mathfrak{g}^{\mathfrak{m}} \hookrightarrow \mathbb{Q}\langle e_0, e_1\rangle$ provides a complete description of relations among motivic MZVs modulo $(\zeta^{\mathfrak{m}}(2))$, and describing all relations among motivic MZVs determines $\mathfrak{g}^{\mathfrak{m}}$, and hence $\mathrm{G}_{\mathcal{MT}(\mathbb{Z})}$. This could then be used in constructing explicit rational elements of the Grothendieck-Teichmuller group via the inclusion

$$U_{\mathcal{MT}(\mathbb{Z})} \subset \mathrm{GRT}_1 \subset \mathrm{DMR}_0,$$

where the final group is Racinet's double shuffle group. These are conjecturally equalities, and proving this is a very classical approach to describing the motivic Galois group. This is equivalent to showing that equality of the corresponding Lie algebras, or that the double shuffle equations, or associator equations describe all relations among motivic multiple zeta values.

1.1.2 Motivation

The Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ inherits two filtrations arising from filtrations on motivic multiple zeta values. The multiple zeta value

$$\zeta(n_1,\ldots,n_r) := \sum_{1\leq k_1<k_2<\cdots<k_r} \frac{1}{k_1^{n_1}\ldots k_r^{n_r}}$$

is said to have *weight* $n_1+\cdots+n_r$ and *depth* r. We can also consider ζ as a function $\mathbb{Q}\langle e_0,e_1\rangle \to \mathbb{C}$ via iterated integrals, as in Proposition 1.2.9.

Example 1.1.2. We define the function $\zeta(w)$ as an integral over the simplex $0\leq t_1\leq \cdots \leq t_{|w|}\leq 1$, of the differential form obtained by identifying e_1 with $\frac{dz}{z-i}$, e.g.

$$\zeta(e_1e_0e_1e_0) := \int_{0\leq t_1\leq t_2\leq t_3\leq t_4\leq 1} \frac{dt_1}{t_1-1}\frac{dt_2}{t_2}\frac{dt_3}{t_3-1}\frac{dt_4}{t_4} = \zeta(2,2).$$

To see that, up to a sign, we obtain a multiple zeta value, we write $\frac{1}{z-1} = -\sum_{n\geq 0} z^n$, and integrate term by term.

As such, we can extend these notions to $\mathbb{Q}\langle e_0,e_1\rangle$, where the weight $|w|$ of a word $w\in\{e_0,e_1\}^\times$ is given by its length, and the depth $d(w)$ of w is the number of occurrences of e_1. Thus we define

$$\mathcal{W}_n\mathbb{Q}\langle e_0,e_1\rangle := \langle w \ : \ |w|\leq n\rangle_{\mathbb{Q}},$$
$$\mathcal{D}_n\mathbb{Q}\langle e_0,e_1\rangle := \langle w \ : \ d(w)\leq n\rangle_{\mathbb{Q}}.$$

These induce increasing filtrations on $\mathcal{H}$ and hence induce decreasing filtrations on $\mathfrak{g}^{\mathfrak{m}}$, given via its embedding into $\mathbb{Q}\langle e_0,e_1\rangle$ (viewed here as the graded dual of $\mathbb{Q}\langle e_0,e_1\rangle$) by

$$\mathcal{W}^n\mathbb{Q}\langle e_0,e_1\rangle := \langle w \ : \ |w|\geq n\rangle_{\mathbb{Q}},$$
$$\mathcal{D}^n\mathbb{Q}\langle e_0,e_1\rangle := \langle w \ : \ d(w)\geq n\rangle_{\mathbb{Q}}.$$

It is known that weight is a grading for $\mathfrak{g}^{\mathfrak{m}}$, but depth is not.

The classical approach to describing elements of $\mathrm{G}_{\mathcal{MT}(\mathbb{Z})}$ has been to solve the double shuffle equations [38] depth by depth. This has been met with some success, such as Brown's solution modulo depth 4 [13], but still proves quite challenging. To further simplify, we can consider depth graded analogues. In [10], Brown studies the associated bigraded vector space $\mathfrak{dg} := \mathrm{gr}_{\mathcal{D}}\mathfrak{g}^{\mathfrak{m}}$ and its embedding into the linearised double shuffle algebra $\mathfrak{ls}$. These describe relations among motivic MZVs modulo products and terms of lower depth.

Example 1.1.3. Classically, it is a standard result that

$$\zeta(2,3) + \zeta(3,2) + \zeta(5) = \zeta(2)\zeta(3),$$

arising from the decomposition of domain of summation as follows

$$\begin{aligned}\zeta(2)\zeta(3) &= \sum_{m\geq 1}\frac{1}{m^2}\sum_{n\geq 1}\frac{1}{n^3}\\ &= \sum_{0<m<n}\frac{1}{m^2n^3} + \sum_{0<n<m}\frac{1}{m^2n^3} + \sum_{m=n>0}\frac{1}{m^5}\\ &= \zeta(2,3) + \zeta(3,2) + \zeta(5)\end{aligned}$$

The depth graded version of this relation, modulo products, is

$$\zeta(2,3) + \zeta(3,2) = 0.$$

This approach has many strengths. Depth is somehow 'motivic', by which we mean it is compatible with the Lie algebra structure on $\mathfrak{g}^{\mathfrak{m}}$. We can thus show that $\mathfrak{dg}$ is in fact a Lie algebra, and the depth 1 part of σ_{2k+1} defines canonical representative of σ_{2k+1} in $\mathfrak{dg} \to \mathbb{Q}\langle e_0, e_1\rangle$. The combinatorics is significantly simplified, and this approach has led to several interesting results regarding totally odd zeta values [18]. Most importantly, there is an explicit description of a conjecturally complete set of relations among depth graded motivic MZVs [33].

Unfortunately there also exist relations in $\mathfrak{dg}$.

Example 1.1.4.

$$\{\sigma_3, \sigma_9\} - 3\{\sigma_5, \sigma_7\} = 0$$

modulo terms of depth three or higher.

Hence 'exceptional' generators are needed. These relations are shown to have a somewhat mysterious connection to period polynomials of modular forms by Pollack [37][26], and this has been further explored by Baumard and Schneps [4]. However, we only have a conjectural description of the dimension of the graded pieces due to Broadhurst-Kreimer, given in terms of the space of cusp forms [7].

Thus this approach is limited by our understanding of this connection to modular forms.

1.1.3 Strategy

In this thesis we propose an alternative approach. We introduce a new increasing motivic filtration on motivic multiple zeta values, which we call the block filtration, based on Charlton's decomposition into alternating blocks [14]. We define this in terms of a combinatorial degree on $\mathbb{Q}\langle e_0, e_1\rangle$.

$$\deg_{\mathcal{B}}(w) := \#\{\text{Occurrences of } e_0e_0 \text{ or } e_1e_1 \text{ in } e_0we_1\}$$

The occurrences of e_i^2 in e_0we_1 divide e_0we_1 into alternating blocks of length $(l_1, \dots, l_{\deg_{\mathcal{B}}(w)+1})$, which we call the *block decomposition* associated to w.

Example 1.1.5.

$$\begin{aligned} \deg_{\mathcal{B}}(e_1e_0e_0) &= 1 \\ \deg_{\mathcal{B}}(e_0e_1e_1e_0) &= 2 \\ \deg_{\mathcal{B}}(e_1e_0e_1e_1e_1e_0) &= 2 \end{aligned}$$

This filtration is very nice to work with: it has a simple description, it is (unlike depth) preserved by the symmetry $\{0\} \leftrightarrow \{1\}$ of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, and we show it agrees with the coradicial filtration defined via the motivic coaction. This suggests that the algebra of block graded multiple zeta values may be a very natural object to consider. Indeed, we have already seen some success with this approach: the block filtration generalises the level filtration on the Hoffman zeta elements, which was instrumental in Brown's proof that the Hoffman zeta elements form a basis for the space of motivic MZVs [9].

We immediately see that many known relations are significantly simplified when considered modulo products and terms of lower block degree.

Example 1.1.6. Recall

$$\zeta(2,3)+\zeta(3,2)+\zeta(5)=\zeta(2)\zeta(3).$$

The block graded version of this relation, modulo products, is

$$\zeta(5)=0.$$

Modulo products, one can show

$$2\zeta(3,3)+\zeta(3,1,2)=\zeta(2,2,2).$$

The block graded version of this is

$$2\zeta(3,3)+\zeta(3,1,2)=0.$$

We find that many MZVs vanish modulo terms of lower block degree. This provides a slight barrier, as many known relations "vanish" in the block graded algebra. However, unlike the depth graded case, the dimension of each graded piece is known explicitly. So if we can find a set of relations, it is simple to check if these are sufficient to describe all relations among block graded multiple zeta values. Furthermore, as a consequence of Theorem 2.2.7, providing a lift of these relations to relations among motivic MZVs will describe all relations among motivic MZVs. Thus we have a clear strategy:

1. Describe all relations among block graded MZVs. Equivalently, explicitly describe $\bigoplus_{n=1}^{\infty}\mathcal{B}^n\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^{n+1}\mathfrak{g}^{\mathfrak{m}}$ as a subset of $\mathbb{Q}\langle e_0,e_1\rangle$.

2. Prove that these relations describe a space of the correct dimension in each block-

graded piece.

3. Lift these relations to genuine relations among motivic MZVs, and explicitly describe the image of $\mathfrak{g}^{\mathfrak{m}}$ in $\mathbb{Q}\langle e_0, e_1\rangle$.

1.1.4 Summary of Results

We have made significant progress towards this goal. Our strategy relies quite explicitly on the following result, shown in Theorem 2.2.7 and Corollary 2.2.8.

Theorem.

$$\mathfrak{g}^{\mathfrak{m}} \cong \bigoplus_{n=1}^{\infty} \mathcal{B}^n\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^{n+1}\mathfrak{g}^{\mathfrak{m}}$$

With this in mind, we move toward step 1 of describing relations. This is very fruitful: for example, we find a new shuffle relation.

Theorem. *Let $I(l_1, \ldots, l_r)$ denote the MZV associated to the block decomposition $(l_1, \ldots, l_r)$ as in Definition 2.3.2 and define*

$$Sh_{k,r-k} := \{\sigma \in S_r \mid \sigma^{-1}(1) < \cdots < \sigma^{-1}(k),\ \sigma^{-1}(k+1) < \cdots < \sigma^{-1}(r)\}.$$

Then for $1 \leq k < r$,

$$\sum_{\sigma \in Sh_{k,r-k}} I(l_{\sigma(1)}, \ldots, l_{\sigma(r)}) = 0$$

modulo products and terms of lower block degree.

Example 1.1.7. Choosing $r = 4,\ k = 1$ and $(l_1, l_2, l_3, l_4) = (4, 3, 4, 2)$, we find that

$$\zeta(2,1,2,1,2,3) + 2\zeta(3,2,1,2,3) + \zeta(3,2,1,3,2) = 0$$

modulo products and terms of lower block degree.

We also find an embedding $\mathcal{B}^n\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^{n+1}\mathfrak{g}^{\mathfrak{m}} \hookrightarrow \mathbb{Q}[x_1, \ldots, x_{n+1}]$, which reveals additional symmetries. We denote the image of this embedding by $\mathfrak{rbg}_n$.

Theorem. *Any $f(x_1, \ldots, x_{n+1}) \in \mathfrak{rbg}_n$ satisfies*

$$f(x_1, \ldots, x_{n+1}) = f(x_2, \ldots, x_{n+1}, x_1) = (-1)^{n+1} f(x_{n+1}, \ldots, x_2, x_1).$$

Furthermore, $\mathfrak{rbg}_n$ is annihilated by the differential operator given in Definition 2.7.1.

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

Promisingly, we can achieve a complete description of all block graded relations in low block degree.

Theorem. *There exist explicit relations completely describing $\mathcal{B}^1\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^2$ and $\mathcal{B}^2\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^3$, giving vector spaces of the correct dimension.*

If these results can be extended beyond block degree 2, this provides a complete description of all relations among block graded MZVs. We have also been able to lift many of these to genuine relations among motivic MZVs.

Example 1.1.8.

$$\zeta(\{2\}^k \sqcup\!\sqcup \{1,3\}^n) = \frac{\pi^{4n+2k}}{(2n+1)(4n+2k+1)!}\binom{2n+k}{k}.$$

This provides significant evidence for validity of this strategy, and establishes new and exciting relations among multiple zeta values.

Additionally, as this project was originally motivated by defining a canonical rational associator we also briefly consider the implication of known relations - specifically the double shuffle relations - on the coefficients of a rational associator. We establish the non-existence of integral solutions, and provide a bound on the p-adic valuation of coefficients. We also establish a partial result deriving a motivic relation from the double shuffle relations.

1.1.5 Outline

In Chapter 1, we will condense the necessary background material. We briefly introduce multiple zeta values, their combinatorics, and their connection to Drinfeld associators. We then introduce three algebraic groups - the double shuffle group, the Grothendieck-Teichmuller group, and the motivic Galois group - and their Lie algebras. Here we shall also introduce motivic multiple zeta values, the motivic coaction, and some results due to Brown.

In Chapter 2, we expand on some of the implications of Brown's motivic machinery, in particular of the motivic coaction. We introduce a new filtration preserved by the coaction - 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 associated to the motivic coaction. We consider the associated graded algebra with respect to this filtration, and describe some new families of relations arising from the Lie algebra. The dual Lie algebra is shown to be isomorphic to the motivic Lie algebra. This isomorphism suggests that many of these graded relations should lift to families of relations among motivic multiple zeta values.

In Chapter 3, we ask whether the relations satisfied by block graded multiple zeta values imply graded versions of known relations, specifically the double shuffle relations and the Ohno-Zagier relations. We conclude that the "obvious" graded relations are indeed consequences of the block relations.

In Chapter 4, we consider the lifts of our block graded relations to relations modulo products. We provide an explicit isomorphism between the shuffle algebra and the block shuffle algebra to establish yet another family of relations modulo products. We then compute the products via combinatorial methods.

In Chapter 5, we consider solutions to the double shuffle equations over fields of positive 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.

In Chapter 6, we present some small observations on an alternative approach to defining canonical generators, and some thoughts on duality as a consequence of the double shuffle relations.

1.2 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 [31] or [41] for a more expository recap. A reader familiar with the material may skip to the next chapter.

Definition 1.2.1. For a sequence of integers $(s_1, \ldots, s_r)$ with $s_i \geq 1$ and $s_r \geq 2$, we define the corresponding multiple zeta value by

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

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

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

Example 1.2.2.

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

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

Definition 1.2.3. Denote a sequence of positive integers $(i_1, \ldots, i_k)$ by the product $y_{i_1} y_{i_2} \ldots y_{i_k}$ in noncommutative formal variables $y_1, y_2, \ldots$. Denote the empty sequence by 1. Given two sequences of integers, $y_{i_1} \ldots y_{i_r}$ and $y_{j_1} \ldots y_{j_q}$, we recursively define their stuffle product as the formal sum obtained from

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

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

Proposition 1.2.4.

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

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 [15].

Definition 1.2.5. Let M be a connected differentiable manifold, and let $\mathcal{P}(M)$ be the set of all paths in M. To be precise, define

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

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

$$\int \omega_1,\omega_2,\dots,\omega_r : \mathcal{P}(M) \to k$$
$$\gamma \mapsto \int_\gamma \omega_1\omega_2,\dots\omega_r$$

given by

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

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

Remark 1.2.6. 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 1.2.7. 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 1.2.8. Similarly to order of integration in iterated integrals, and order of summation in MZVs, there is no standard convention for these ω_i. It is quite common to have this defined as

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

We will exclusively use Definition 1.2.7.

Proposition 1.2.9. *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* ω_w *along the straight line path between* 0 *and* 1

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

Example 1.2.10. Let $w := 100$, then the iterated integral of ω_w is given by

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

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 1.2.11.

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

To make this precise, we consider ζ 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:

$$\zeta(e_1e_0^{s_1-1}e_1\dots e_1e_0^{s_r-1}) = \zeta(s_1,\dots,s_r)$$

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

Definition 1.2.12. Given two elements of $\mathbb{Q}\langle e_0,e_1\rangle$, define their shuffle product recursively by

$$1ш u = uш 1 = u,$$

$$xuш yv = x(uш yv)+y(xuш v)$$

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

Proposition 1.2.13. *For any monomials u,v in $e_1\mathbb{Q}\langle e_0,e_1\rangle e_0$, we have*

$$\zeta(uш v)=\zeta(u)\zeta(v).$$

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

Proposition 1.2.14. *Let $D:\mathbb{Q}\langle e_0,e_1\rangle\to\mathbb{Q}\langle e_0,e_1\rangle$ 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 ζ to a function on all of $\mathbb{Q}\langle e_0, e_1\rangle$ [33]. For example, we can define shuffle regularised iterated integrals as follows.

Definition 1.2.15. For a word $w = e_0^n e_1 e_0^{n_1} e_1 \dots e_1 e_0^{n_r}$, define $\zeta(w)$ by the sum

$$\zeta(w) = -\sum_{\substack{k_1+\ldots+k_r=n \\ k_1,\ldots,k_r\geq 0}} \prod_{i=1}^{r} \binom{n_i+k_i}{k_i} \zeta(e_1 e_0^{n_1+k_1} e_1 e_0^{n_2+k_2} \dots e_1 e_0^{n_r+k_r}).$$

By application of this formula, and Proposition 1.2.14, we can uniquely associated a sum of convergent multiple zeta values to any word w in $\{e_0, e_1\}$.

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 1.2.16. $\mathcal{Z}$ 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 $\zeta(\varnothing) = 1$.

Conjecture 1.2.17. 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 1.2.18. All relations among multiple zeta values can be obtained from the shuffle and stuffle relations, alongside the Hoffman relation:

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

for all convergent u.

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

As discussed in the introduction, our goal is to describe the motivic Galois group of mixed Tate motives via relations among multiple zeta values. We now review the definitions of the motivic Galois group and motivic multiple zeta values. As general references, the works of Ayoub [2], Deligne [17] and Brown [11], [9] can be useful.

Let $\mathcal{MT}(\mathbb{Z})$ denote the category of mixed Tate motives unramified over $\mathbb{Z}$. This is a (neutral) Tannakian category over $\mathbb{Q}$, which is to say it is a rigid abelian tensor category with an exact faithful $\mathbb{Q}$-linear tensor functor - the fiber functor - to the category of finite dimensional $\mathbb{Q}$-vector spaces. It is hence equivalent to the category of representations of a group scheme, called its Galois group and denoted by $G_{\mathcal{MT}(\mathbb{Z})}$. Explicitly, if ω_{dR} is the fiber functor, $G_{\mathcal{MT}(\mathbb{Z})}$ is defined to be $\underline{Aut}^{\otimes}(\omega_{dR})$, the group scheme of tensor automorphisms of the fiber functor. $\mathcal{MT}(\mathbb{Z})$ 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

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

Remark 1.2.19. In [9], Brown shows this map is in fact an isomorphism. As such, we will often identify $\mathcal{MT}'(\mathbb{Z})$ with $\mathcal{MT}(\mathbb{Z})$.

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. For a more precise definition, we refer the reader to Deligne [16]

Definition 1.2.20. Let $T_{(0,1,\infty)}(X)$ be the set of tangent vectors to X at $\{0,1,\infty\}$, in the sense of Deligne [16]. The motivic fundamental groupoid of X consists of the following data.

- (Betti) A scheme $\pi_1^B(X,x,y)$ defined over $\mathbb{Q}$ for every $x, y \in X(\mathbb{C}) \cup T_{(0,1,\infty)}(X)$ such that the collection is equipped with the structure of a groupoid

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

  for any $x, y, z \in X(\mathbb{C}) \cup T_{(0,1,\infty)}(X)$ and such that there exists a natural homomorphism

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

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 $\mathbb{Q}$ for every $x, y \in X(\mathbb{C}) \cup T_{(0,1,\infty)}$, denoted by $\pi_1^{dR}(X, x, y)$. This is independent of choice of basepoints, so we often write $\pi_1^{dR}(X)$ instead. It is the Tannakian Galois group of the category of unipotent vector bundles over X with integrable connection.

- (Comparison) For every $x, y \in X(\mathbb{C}) \cup T_{(0,1,\infty)}$, a canonical isomorphism of schemes over $\mathbb{C}$
$$\mathrm{comp} : \pi_1^B(X, x, y) \times_{\mathbb{Q}} \mathbb{C} \to \pi_1^{dR}(X) \times_{\mathbb{Q}} \mathbb{C}.$$

Remark 1.2.21. We gloss over the technicalities of tangential basepoints [16]. 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 $\gamma : (0, 1) \to \mathbb{C} \setminus \{0, 1\}$ with $\gamma(0) = 0$, $\gamma(1) = 1$ in the following discussion have $\gamma'(0) = \gamma'(1) = 1$.

Theorem 1.2.22. *There is an ind-object*

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

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 ${}_0\Pi_1 := \mathrm{Spec}(\mathcal{O}(\pi_1^{dR}(X)))$. 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

$$\{S \in R\langle\langle e_0, e_1\rangle\rangle | \Delta S = S \otimes S \text{ and } S \text{ has constant term } 1\}$$

where Δ is the completed coproduct for which e_i are primitive. This carries an action of the motivic Galois group $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$, which depends on our choice of basepoints, even though $\pi_1^{dR}(X)$ does not contain an explicit dependence on these points.

Remark 1.2.23. 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 1.2.20 maps dch onto an element ${}_01_1^B \in \pi_1^B(X, 0, 1)(\mathbb{Q})$. The image of this map under the comparison isomorphism is called the KZ associator

$$\operatorname{comp}({}_01_1^B) = \sum_w \zeta(w)w \in {}_0\Pi_1(\mathbb{C}).$$

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

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

which factors through a map

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

called the Ihara action, computed explicitly first by Y. Ihara, but described in [17].

Remark 1.2.24. We later introduce the *linearised*, or *infinitesimal* Ihara action, in the context of the Lie algebras of DMR_0 and $U_{\mathcal{MT}(\mathbb{Z})}$. We will almost exclusively refer to this linearised Ihara action, rather than the group law.

1.2.2 Motivic multiple zeta values

To the preceding groups, we can associate a ring of motivic periods, as in [11]. Given two fiber functors $\omega_B, \omega_{dR} : \mathcal{MT}(\mathbb{Z}) \to \mathrm{Vec}_{\mathbb{Q}}$, we define the ring of motivic periods

$$\mathcal{P}^{\mathfrak{m}}_{\mathcal{MT}(\mathbb{Z})} = \mathcal{O}(\underline{Isom}^{\otimes}(\omega_{dR}, \omega_B)).$$

Every motivic period can be represented as a triple, consisting of an object $M \in \mathcal{MT}(\mathbb{Z})$, and a pair of elements $w \in \omega_{dR}(M)$ and $\sigma \in \omega_B(M)^\vee$, which we write as $[M, w, \sigma]^{\mathfrak{m}}$.

Denote by $\mathcal{O}({}_x\Pi^{\mathfrak{m}}_y)$ the affine ring of the motivic fundamental groupoid of $\mathbb{P}^1 \setminus \{0,1,\infty\}$. Considering motivic periods with $M = \mathcal{O}({}_x\Pi^{\mathfrak{m}}_y)$, we obtain our first definition of motivic iterated integrals and motivic multiple zeta values.

Definition 1.2.25. Define the motivic multiple zeta value associated to the word w in $\{0,1\}$ to be the motivic period

$$\mathrm{I}^{\mathfrak{m}}(x;w;y) = [\mathcal{O}({}_x\Pi^{\mathfrak{m}}_y), w, {}_x1^B_y]^{\mathfrak{m}} \in \mathcal{P}^{\mathfrak{m}}_{\mathcal{MT}(\mathbb{Z})}$$

where ${}_x1^B_y \in \mathcal{O}(\pi_1^B(X,x,y))^\vee$ are the images of the paths

$$dch \text{ if } (x,y)=(0,1);\; dch^{-1} \text{ if } (x,y)=(1,0);\; c_x, \text{ the constant path at } x, \text{ if } x=y.$$

Denote by $\mathcal{H}$ the algebra of motivic multiple zeta values.

By considering triples $[\mathcal{O}({}_x\Pi^{\mathfrak{m}}_y), w, {}_x1^{dR}_y]^\vee$, where ${}_x1^{dR}_y \in \mathcal{O}({}_x\Pi^{dR}_1)$ is given by projection onto weight 0, we obtain elements of $\mathcal{O}(\underline{Isom}^{\otimes}(\omega_{dR},\omega_{dR}))$. We call these *de Rham* multiple zeta values. The de Rham multiple zeta value associated to the word w in $\{0,1\}$ is denoted by $\mathrm{I}^{\mathfrak{a}}(x;w;y)$, and we define $\mathcal{A}$ to be the algebra of de Rham multiple zeta values. In a slight abuse of notation, we will also introduce $\zeta^{\mathfrak{m}}(w)$ and $\zeta^{\mathfrak{a}}(w)$ which are defined by

$$\zeta^\bullet(w) := (-1)^{d(w)}\mathrm{I}^\bullet(0;w;1).$$

Remark 1.2.26. One can define a naive map $\mathcal{H} \to \mathcal{A}$ sending $\mathrm{I}^{\mathfrak{m}}(x;w;y) \mapsto \mathrm{I}^{\mathfrak{a}}(x;w;y)$. This can be shown to be well defined, with kernel equal to the ideal generated by $\zeta^{\mathfrak{m}}(2)$.

With these definitions, the existence of an action

$$U^{dR}_{\mathcal{MT}(\mathbb{Z})} \times {}_0\Pi_1 \to {}_0\Pi_1$$

is apparent. This action dualises to a coaction

$$\Delta : \mathcal{O}({}_0\Pi_1) \to \mathcal{O}(U^{dR}_{\mathcal{MT}(\mathbb{Z})}) \otimes \mathcal{O}({}_0\Pi_1)$$

which gives a coaction

$$\Delta : \mathcal{H} \to \mathcal{A} \otimes \mathcal{H}.$$

This has an explicit formula, initially due to Goncharov [27], who computed the corresponding coproduct

$$\Delta : \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}.$$

This was later extended by Brown to the following explicit coaction [9].

Proposition 1.2.27. *The motivic coaction $\Delta : \mathcal{H} \to \mathcal{A} \otimes \mathcal{H}$ is given by the following formula.*

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

With this coaction in mind, we can provide an alternative, more concrete definition of motivic multiple zeta values.

Definition 1.2.28. Define a period map from $\mathcal{O}({}_0\Pi_1) \to \mathbb{C}$ by taking the associated iterated integral: $e_{a_1} \dots e_{a_n} \mapsto \mathrm{I}(0; a_1, \dots, a_n; 1)$, and denote by $\mathcal{J} \subset \mathcal{O}({}_0\Pi_1)$ the largest ideal contained in the kernel of this period map that is stable under Δ. We define

$$\mathcal{H} := \mathcal{O}({}_0\Pi_1)/\mathcal{J}$$

and let $\mathrm{I}^{\mathfrak{m}}(0; a_1, \dots, a_n; 1)$ denote the image of $e_{a_1} \dots e_{a_n}$ in $\mathcal{H}$.

We can then define $\mathcal{A} := \mathcal{H}/(\zeta^{\mathfrak{m}}(2))$.

Remark 1.2.29. Note that it is a nontrivial task to show equivalence of these definitions. However, this is well established in the literature, and we will not focus too much on this detail.

This coaction is a very powerful computational tool. It somehow encodes all motivic relations, best illustrated in a theorem due to Brown [9], given below. First, we introduce the infinitesimal coactions: a family of maps through which the motivic coaction factors that are easier to compute.

Definition 1.2.30. Let $\mathcal{A}_{>0}$ be the subspace of $\mathcal{A}$ spanned by elements of positive weight. Define the Lie coalgebra of indecomposables to be $\mathcal{L} := \mathcal{A}_{>0}/\mathcal{A}_{>0}\mathcal{A}_{>0}$, and denote by $\mathrm{I}^{\mathfrak{l}}(x;w;y)$ the image of $\mathrm{I}^{\mathfrak{a}}(x;w;y)$ in $\mathcal{L}$. Then, for every $r > 0$, define the infinitesimal coaction

$$D_{2r+1} : \mathcal{H} \to \mathcal{L} \otimes \mathcal{H}$$

as the derivation given by

$$\begin{aligned} &D_{2r+1}\mathrm{I}^{\mathfrak{m}}(0; a_1, \dots, a_n; 1) = \\ &\sum_{k=0}^{n-2r-1} \mathrm{I}^{\mathfrak{l}}(a_i; a_{i+1}, \dots, a_{i+2r+1}; a_{i+2r+2}) \otimes \mathrm{I}^{\mathfrak{m}}(a_0; a_1, \dots, a_i, a_{i+2r+2}, \dots, a_n; a_{n+1}). \end{aligned}$$

Then, Brown tells us that the following holds.

Theorem 1.2.31. *Let $\mathcal{H}_N$ be the subspace of $\mathcal{H}$ spanned by elements of weight N. Then*

$$\mathcal{H} \cap ker\Big(\bigoplus_{3 \le 2r+1 < N} D_{2r+1}\Big) = \mathbb{Q}\zeta^{\mathfrak{m}}(N).$$

This provides a powerful tool for finding and verifying relations among multiple zeta values of motivic origin.

1.3 The double shuffle equations

While the theory of motives provides a powerful tool for producing relations among motivic MZVs, it does not give us an explicit spanning set of relations, and so we cannot easily describe elements of the motivic Galois group. In attempting to provide such an explicit description, we can consider conjecturally complete sets of relations. The simplest of these are the double shuffle relations, arising from the double algebra structure on $\mathcal{Z}$. Following the work of Racinet [38], we define a group scheme containing $G_{\mathcal{MT}(\mathbb{Z})}$. Let k be a field. It need not be of characteristic zero, but is normally taken to be.

Definition 1.3.1. We say a power series $\Phi \in k\langle\langle e_0, e_1 \rangle\rangle$ solves the shuffle equations if it is grouplike for the completed coproduct for which e_0, e_1 are primitive. That is, Φ has constant coefficient 1 and

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

where

$$\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i \text{ for } i \in \{0, 1\}.$$

Definition 1.3.2. Let $Y = y_1, y_2, y_3, \ldots$ 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 1.3.3. Define the projection map $\pi_Y : k\langle\langle e_0, e_1\rangle\rangle \to k\langle\langle Y\rangle\rangle$ to be the linear map given by

$$\pi_Y(e_1 e_0^{n_1-1} e_1 e_0^{n_2-1} \ldots e_1 e_0^{n_k-1}) = y_{n_1} y_{n_2} \cdots y_{n_k}$$

and $\pi_Y(e_0 w) = 0$ for any word $w \in k\langle e_0, e_1\rangle$. Define also, for any element $\Phi \in k\langle\langle a, b\rangle\rangle$, $\Phi_{corr} \in k\langle\langle Y\rangle\rangle$ by

$$\Phi_{corr} := \exp(\sum_{n\geq 1} \frac{(-1)^n}{n} (\Phi | e_1 e_0^{n-1}) y_1^n)$$

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

Definition 1.3.4. We say a power series $\Phi \in k\langle\langle e_0, e_1\rangle\rangle$ solves the (regularised) double shuffle equations if Φ solves the shuffle equations and $\Phi^* := \Phi_{corr}\pi_Y(\Phi)$ solves the stuffle equations.

Then, the statement that multiple zeta values satisfy the double shuffle relations is precisely the statement that

$$\Phi := 1 + \sum_{w \in \{e_0, e_1\}} \zeta(w) w$$

solves the double shuffle equations. The space of solutions to the double shuffle equations, denoted DMR, contains a subspace of solutions, DMR_0, such that $(\Phi|e_0) = (\Phi|e_1) = (\Phi|e_0 e_1) = 0$. This subspace forms a pro-unipotent group [38] with multiplication given by

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

It is known [38] that

$$U_{\mathcal{MT}(\mathbb{Z})} \subset \mathrm{DMR}_0$$

and it is a standard conjecture this is an equality. However, studying DMR_0 is much simpler that $G_{\mathcal{MT}(\mathbb{Z})}$: it is described by explicit, simple relations that behave well with respect to the weight and depth filtrations. Additionally, the double shuffle equations lend themselves well to a rewriting in terms of commutative power series, a technique used extensively by Brown, and very similar to Écalle's theory of moulds [20]. This technique has allowed Brown to define a canonical rational associator up to depth 4.

Remark 1.3.5. From this point in the text, we are interested primarily in DMR_0, and so we shall assume $(\Phi|e_0) = (\Phi|e_1) = (\Phi|e_0e_1) = 0$ for all potential solutions to the shuffle or stuffle equations.

Definition 1.3.6. Denote by D_n the vector space spanned by words of depth n in $k\langle e_0, e_1\rangle$ and let $\rho_n : D_n \to k[[y_0, y_1, \ldots, y_n]]$ be the isomorphism of vector spaces given by

$$\rho_n(e_0^{m_0} e_1 e_0^{m_1} \ldots e_1 e_0^{m_n}) = y_0^{m_0} y_1^{m_1} \ldots y_n^{m_n}.$$

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

$$\rho : k\langle e_0, e_1\rangle \to \bigoplus_{n=1}^{\infty} k[y_0, \ldots y_n]$$
$$\Phi \mapsto \{\Phi^{(n)}(y_0, \ldots, y_n)\}_{n=1}^{\infty}.$$

We can then define the double shuffle equations in this new formulation as polynomial equations. First we note the following lemma.

Lemma 1.3.7. *If $\Phi = 1 + \Phi_1 + \Phi_2 + \ldots$ solves the shuffle equations, where Φ_n is the depth n component of Φ, then $\rho_n(\Phi_n) \in k[y_0, \ldots, y_n]$ is translation invariant.*

Proof. Define $\delta : k\langle e_0, e_1\rangle \to k\langle e_0, e_1\rangle$ to be the derivation given on generators by

$$\delta(e_0) := 1,$$
$$\delta(e_1) := 0.$$

Note that

$$\delta(e_0^{m_0}e_1e_0^{m_1}\dots e_1e_0^{m_k}) = \sum_{i=0}^{k} m_i e_0^{m_0}e_1e_0^{m_1}\dots e_1e_0^{m_i-1}\dots e_1e_0^{m_k}$$

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 δ 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.

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

That is, we will use y_i as variables for the image of ρ, 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 1.3.8. 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

$$f(\boldsymbol{x}_1\dots\boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+1}\dots\boldsymbol{x}_n) := f(\boldsymbol{x}_1, (\boldsymbol{x}_2\dots\boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+1}\dots\boldsymbol{x}_n)) + f(\boldsymbol{x}_{j+1}, (\boldsymbol{x}_1\dots\boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+2}\dots\boldsymbol{x}_n))$$

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

Definition 1.3.9. We say a family of polynomials $\{f^{(n)}\}$ solves the shuffle equations if

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

for all $1 \leq j < n$.

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

Definition 1.3.10. For any family of polynomials $\{f^{(n)}\}$, define the operators

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

Definition 1.3.11. Define recursively

$$\begin{aligned} f^{(r)}(1 \star \boldsymbol{x}_1 \dots \boldsymbol{x}_r) = f^{(r)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_r \star 1) &= f^{(r)}(x_1, \dots, x_r), \\ f^{(r)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+1} \dots \boldsymbol{x}_r) &= s_1 f^{(r-1)}(\boldsymbol{x}_2 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+1} \dots \boldsymbol{x}_r) \\ &\quad + s_{i+1} f^{(r-1)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+2} \dots \boldsymbol{x}_r) \\ &\quad + \left(\frac{s_1 - s_{i+1}}{x_1 - x_{i+1}} \right) f^{(r-2)}(\boldsymbol{x}_2 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+2} \dots \boldsymbol{x}_r) \end{aligned}$$

where $1 \leq i \leq r$.

Definition 1.3.12. We say a family of polynomials $\{f^{(n)}\}$ solves the stuffle equations if

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

for all $1 \leq j < n$.

Remark 1.3.13. Note that in this formulation, there is no mention of an analogue to Φ_{corr}. It is true that we must add a corresponding correction term, given by

$$f_{corr}^{(n)} = \frac{(-1)^n}{n!} \left(\sum_{r \geq 1} \sum_{k_1 + \dots + k_r = n} \prod_{i=1}^{r} \frac{c_{k_i}(f)}{k_i} \right) x_1 x_2 \dots x_n$$

where $c_n(f)$ denotes the coefficient of x_1^n in $f^{(1)}$ Denote by $\{f^(n)_\bullet\}$ the family of polynomials $\{f^{(n)} + f_{corr}^{(n)}\}$.

Example 1.3.14. In depth 2, the double shuffle equations are

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

while in depth 3, they become

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

Remark 1.3.15. 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.

These provide powerful computational tools for studying the motivic Galois group.

1.4 Drinfeld associators and the KZ equations

MZVs additionally satisfy relations coming from the theory of associators. In his 1990 work [19] Drinfeld introduced these power series in two non-commuting variables, arising from a study of braided monoidal categories.

Definition 1.4.1. Let k be a field of characteristic 0 and $\lambda \neq 0 \in k$. A *λ-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

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

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

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

$$t_{ii} = 0,$$

$$t_{ij} = t_{ji},$$

$$[t_{ij}, t_{kl}] = 0 \text{ if i, j, k, l distinct,}$$

$$[t_{ij}, t_{ik} + t_{jk}] = 0 \text{ if i, j, k distinct.}$$

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

Interestingly, the hexagon equations are, to some extent, unnecessary, as shown by Furusho [24].

Theorem 1.4.2 (Furusho). *Let Φ be a grouplike power series in two non commuting variables, satisfying Drinfeld's pentagon equation. Then there is a unique λ, depending only on the coefficient of the degree 2 terms, such that the pair (λ, Φ) 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 [3], quantum field theory and deformation-quantisation [34], 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 1.4.3. Define the Grothendieck-Teichmüller group GT to be the affine group scheme over $\mathbb{Q}$, whose k points are given by pairs (λ, f) in $k^\times \times k\langle\langle x, y\rangle\rangle$ such that

$$\Delta f = f \hat{\otimes} f,$$

$$f(y,x) = f(x,y)^{-1},$$

$$f(z,x)z^{\frac{\lambda-1}{2}} f(y,z) y^{\frac{\lambda-1}{2}} f(x,y) x^{\frac{\lambda-1}{2}} = 1,$$

$$f(x_{12}, x_{23}x_{24}) f(x_{13}x_{23}, x_{34}) = f(x_{23}, x_{34}) f(x_{12}x_{13}, x_{24}x_{34}) f(x_{12}, x_{23}),$$

where $xyz = 1$ and x_{ij} are elements of the pure braid group, and Δ 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 1.4.4. The coefficient of $e_0 e_1$ in f nearly determines λ. 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 graded Grothendieck-Teichmüller group GRT. GRT_1 is the space of power series $\Phi \in k\langle\langle e_0, e_1\rangle\rangle$ solving the equations of Definition 1.4.1 with $\lambda = 0$, the space of '0-associators. $\mathrm{GRT} := k^\times \ltimes \mathrm{GRT}_1$ with $\mu \cdot \Phi(e_0, e_1) := \Phi(\mu e_0, \mu e_1)$, with product defined by

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

which the reader will note is identical to that of DMR_0. We have the following result due to Furusho [25].

Theorem 1.4.5. *Let Φ be a grouplike power series in two noncommuting variable. Suppose also that it satisfies the pentagon equation. Then Φ solves the double shuffle equations.*

This has the immediate corollary.

Corollary 1.4.6. *GRT_1 is a subgroup of DMR_0*

In fact, we have the chain of inclusions (conjecturally equalities)

$$U_{\mathcal{MT}(\mathbb{Z})} \subset \mathrm{GRT}_1 \subset \mathrm{DMR}_0.$$

Thus, by studying associators, in particular 0-associators, we can gain information about $G_{\mathcal{MT}(\mathbb{Z})}$.

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 λ. Drinfeld in fact showed a solution existed and constructed it explicitly [19] from the monodromy of the Knizhnik-Zamolodchikov equations. Its coefficients were later evaluated by Le and Murakami [35], giving the following result.

Theorem 1.4.7. *There exists a solution to the associator equations, called the KZ associator, 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 is the KZ associator obtained as the image of the path *dch* in $G_{\mathcal{MT}(\mathbb{Z})}$. We direct the interested reader to the discussion of [39] for a derivation of the KZ associator via the Knizhnik Zamolodchikov equations. We also have the following interesting corollary.

Corollary 1.4.8. *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 Drinfeld original work [19], or, if the reader is comfortable with braid theoretic language, Bar-Natan's constructive proof [3].

Sketch. It is known that $\mathrm{GRT} \cong \mathbb{G}_m \ltimes \mathrm{GRT}_1$, with GRT_1 a prounipotent 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.

A rational associator is a powerful computational tool, allowing constructions of certain categories and universal knot invariants. Similarly, an explicit rational element of GRT would be a prime candidate for an explicit element of $G_{\mathcal{MT}(\mathbb{Z})}(\mathbb{Q})$.

1.5 The motivic Lie algebra

In order to further simplify computation, we can, instead of considering the inclusion of pro-unipotent groups

$$U_{\mathcal{MT}(\mathbb{Z})} \subset \mathrm{GRT}_1 \subset \mathrm{DMR}_0$$

consider the inclusion of their graded Lie algebras

$$\mathfrak{g}^{\mathfrak{m}} \subset \mathfrak{grt} \subset \mathfrak{dmr}_0 \subset \mathbb{Q}\langle e_0, e_1 \rangle$$

equipped with the Ihara bracket [38].

Definition 1.5.1. Given $\psi \in \mathbb{Q}\langle e_0, e_1 \rangle$, define the derivation $d_\psi : \mathbb{Q}\langle e_0, e_1 \rangle \to \mathbb{Q}\langle e_0, e_1 \rangle$ by

$$\begin{aligned} d_\psi(e_0) &= 0, \\ d_\psi(e_1) &= [e_1, \psi], \end{aligned}$$

where $[u, v] := uv - vu$ is the standard Lie bracket on $\mathbb{Q}\langle e_0, e_1 \rangle$. We define the Ihara bracket $\{\cdot, \cdot\} : \wedge^2 \mathbb{Q}\langle e_0, e_1 \rangle \to \mathbb{Q}\langle e_0, e_1 \rangle$ by

$$\{\psi_1, \psi_2\} := d_{\psi_2}\psi_1 - d_{\psi_1}\psi_2 - [\psi_1, \psi_2].$$

Alternatively, we can define the Ihara bracket via the linearised Ihara action [10].

Definition 1.5.2. Define the linearised Ihara action $\circ : \mathbb{Q}\langle e_0, e_1 \rangle \otimes \mathbb{Q}\langle e_0, e_1 \rangle \to \mathbb{Q}\langle e_0, e_1 \rangle$ on monomials by

$$u \circ e_0^n e_1 v := e_0^n u e_1 v + e_0^n e_1 u^* v + e_0^n e_1 (u \circ v)$$

where $(u_1 u_2 \dots u_r)* = (-1)^r u_r \dots u_1$ and $u \circ e_0^n = e_0^n u$, for all u, v monomials in $\mathbb{Q}\langle e_0, e_1 \rangle$. We extend this linearly to all of $\mathbb{Q}\langle e_0, e_1 \rangle$. Define the Ihara bracket by

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

As the motivic relations, associator relations, and double shuffle relations are all weight graded, so too are the corresponding Lie algebras. It is therefore sufficient to establish equality of their weight graded pieces as finite dimensional vector spaces. This is a much more approachable task, and has been verified numerically to high weight.

It is a standard fact from the theory of mixed Tate motives that $\mathfrak{g}^{\mathfrak{m}} := \mathrm{grLie}(U_{\mathcal{MT}(\mathbb{Z})})$ is non-canonically isomorphic to the free Lie algebra $\mathrm{Lie}[\sigma_3, \sigma_5, \sigma_7, \ldots]$, with a generator in each odd weight greater than 1 [17]. As this isomorphism not canonical, there is no canonical representation of these σ_{2k+1} in $\mathbb{Q}\langle e_0, e_1\rangle$. We have that

$$\sigma_{2n+1} = \mathrm{ad}^{2n}(e_0)(e_1) + \text{ terms of higher depth}$$

where the adjoint action is with respect to the Lie bracket $[X, Y] = XY - YX$. However, given an embedding

$$\{\sigma_{2n+1}\}_{n\geq 1} \hookrightarrow \mathbb{Q}\langle e_0, e_1\rangle,$$

we can replace σ_{2n+1} with $\sigma_{2n+1} + \phi$, for $\phi \in \{\mathfrak{g}^{\mathfrak{m}}, \mathfrak{g}^{\mathfrak{m}}\}$ of weight $2n+1$, and obtain the same Lie algebra. Thus the σ_{2n+1} are ambiguous, limiting their computational use.

Nevertheless, we can still attempt to describe $\mathfrak{g}^{\mathfrak{m}}$ via it's inclusion into $\mathfrak{grt}$ and $\mathfrak{dmr}_0$.

Definition 1.5.3. $\psi(e_0, e_1) \in \mathfrak{grt}$ if and only if ψ satisfies

$$\begin{gathered}\Delta\psi = \psi \otimes 1 + 1 \otimes \psi,\\ \psi(e_1, e_0) = -\psi(e_0, e_1),\\ \psi(-e_1 - e_0, e_0) + \psi(e_1, -e_1 - e_0) - \psi(e_0, e_1) = 0,\\ \psi(x_{12}, x_{23}x_{24}) + \psi(x_{13}x_{23}, x_{34}) = \psi(x_{23}, x_{34}) + \psi(x_{12}x_{13}, x_{24}x_{34}) + \psi(x_{12}, x_{23}),\end{gathered}$$

where $\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i$, and the $x_{i,j}$ are as before.

Remark 1.5.4. If we were interested in complex points of these Lie algebras, the inclusion $\mathfrak{g}^{\mathfrak{m}} \subset \mathfrak{grt}$ can be used to define inexplicit canonical σ-elements: these exists an element of GRT which acts to take the Drinfeld $2\pi i$-associator to it's conjugate $-2\pi i$-associator. This acts non-trivially on $\zeta(2n+1)$, and the weight graded pieces of the logarithm define non-trivial complex σ_{2n+1}. However, this is not a rationally defined construction, and so does not solve the problem of finding a canonical injection $\{\sigma_{2n+1}\}_{k\geq 1} \hookrightarrow \mathbb{Q}\langle e_0, e_1\rangle$.

We can similarly define $\mathfrak{dmr}_0$ as an explicit subset of $\mathbb{Q}\langle e_0, e_1\rangle$.

Definition 1.5.5. We say $\sigma \in \mathbb{Q}\langle e_0, e_1 \rangle$ solves the double shuffle equations mod products if the following hold

$$\begin{aligned} \Delta\sigma &= \sigma \otimes 1 + 1 \otimes \sigma, \\ \Delta_*(\sigma^*) &= \sigma^* \otimes 1 + 1 \otimes \sigma^*, \\ (\sigma|e_0) &= (\sigma|e_1) = (\sigma|e_0e_1) = 0, \end{aligned}$$

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

As before, we may translate this into a statement about commutative polynomials.

Example 1.5.6. In terms of commutative polynomials, the double shuffle equations modulo products are given in depth 2 by

$$\begin{aligned} f^{(2)}(x_1, x_1 + x_2) + f^{(2)}(x_2, x_1 + x_2) &= 0, \\ f_\bullet^{(2)}(x_1, x_2) + f_\bullet^{(2)}(x_2, x_1) + \frac{f_\bullet^{(1)}(x_1) - f_\bullet^{(1)}(x_2)}{x_1 - x_2} &= 0, \end{aligned}$$

Note that, if we assume f to be homogeneous in weight, the correction term only appears in maximal depth, and so can be largely ignored when the weight is greater than the depth.

Chapter 2

The block filtration and block graded multiple zeta values

2.1 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 [14]. 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 2.1.1. 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 2.1.2. Note that, unlike depth, the block degree of a word is preserved by the duality anti-homomorphism mapping $e_i \mapsto e_{1-i}$, 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 [8], 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

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

Brown goes on to show the following.

Proposition 2.1.3 (Brown)**.** *Let $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$ denote the de Rham motivic Galois group of the category $\mathcal{MT}(\mathbb{Z})$, and let $U^{dR}_{\mathcal{MT}(\mathbb{Z})}$ denote its unipotent radical. Then $\mathcal{B}_n$ is stable under the action of $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$, and $U^{dR}_{\mathcal{MT}(\mathbb{Z})}$ acts trivially on $gr^{\mathcal{B}}\mathcal{H}$. Equivalently*

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

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

Corollary 2.1.4 (Brown)**.** *The block filtration induces the level filtration on the subspace spanned by the Hoffman motivic multiple zeta values $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$, with $n_i \in \{2,3\}$, where the level is the number of indices equal to* 3*.*

Proof. The word corresponding to $(n_1, \ldots, n_r)$, with $n_i \in \{2,3\}$ of level m has exactly m occurrences of the subsequence e_0e_0 and none of e_1e_1. Therefore, its block degree is exactly m. Furthermore, since the $\delta_{2r+1,\ell}$ operators introduced in Definition 5.7 of [9] are shown in Proposition 2.1.3 to reduce block degree, we must have that a composition of $m+1$ such operators annihilates any element of block degree m. Since these are known to be injective and level reducing, this implies any element of block degree m is a sum of elements of level at most m. □

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

Corollary 2.1.5 (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*

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

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 $\mathrm{gr}^{\mathcal{B}}\mathcal{H}$ becomes nearly trivial. If we instead extend the filtration as follows, we obtain a much more interesting structure.

Definition 2.1.6. 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 2.1.7.

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

where $\Delta^r(x) = \Delta(x) - \pi_{\mathcal{A}}(x) \otimes 1 - 1 \otimes x$ is the reduced coaction and $\pi_{\mathcal{A}} : \mathcal{H} \to \mathcal{A}$ is the natural projection.

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

$$\mathcal{I} \to \mathcal{H},$$
$$\mathrm{I}^{\mathfrak{f}}(0; w; 1) \mapsto \mathrm{I}^{\mathfrak{m}}(0; w; 1)$$

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

Recall that the motivic coaction is given by the formula

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

where $0 \leq k \leq n$. The infinitesimal coactions are given by

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

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 $\mathcal{I} \to \mathcal{I} \otimes \mathcal{I}$, by calculating these purely symbolically.

Define $\mathcal{I}_n := \langle \mathrm{I}^{\mathfrak{f}}(0; w; 1) \ : \ \deg_{\mathcal{B}}(0w1) = n \rangle_{\mathbb{Q}}$. 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

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

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

$$\mathrm{I}^{\mathfrak{f}}(x; b_i'' b_{i+1} \ldots b_{i+j}'; y) \otimes \mathrm{I}^{\mathfrak{f}}(b_1 \ldots b_{i-1} b_i' x y b_{i+j}'' b_{i+j+1} \ldots b_{n+1})$$

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

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

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

Corollary 2.1.8. *The block filtration on $\mathbb{Q}\langle e_0, e_1\rangle$ induces the coradical filtration on $\mathcal{H}$.*

Proposition 2.1.9. *For all $r \geq 1$, the (linearised) Ihara action $\circ : \mathit{Lie}[e_0, e_1]_{2r+1} \otimes \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle e_0, e_1\rangle$ is graded for block degree, where $\mathit{Lie}[e_0, e_1]_{2r+1}$ denotes Lie polynomials of degree $2r+1$.*

Proof. The Ihara action is dual to the motivic coaction. The linearised Ihara action

$$\circ : \mathrm{Lie}[e_0, e_1]_{2r+1} \otimes \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle e_0, e_1\rangle$$

is dual to the infinitesimal coaction

$$D_{2r+1} : \mathcal{H} \to \mathcal{L} \otimes \mathcal{H}$$

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 [12] for the linearised Ihara action. For example, one must have

$$\begin{aligned}\sigma \circ e_1 e_0^{k_1} \dots e_1 e_0^{k_r} &= \sum_{i=1}^{r+1} e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} \sigma e_1 e_0^{k_i} \dots e_1 e_0^{k_r} \\ &+ \sum_{i=1}^{r} e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} e_1 \sigma^* e_0^{k_i} \dots e_1 e_0^{k_r},\end{aligned}$$

where $(w_1 \dots w_n)^* = (-1)^n w_n \dots w_1$. Since $\sigma \in \mathrm{Lie}[e_0, e_1]$, one must have $\sigma + \sigma^* = 0$, and so

$$\begin{aligned}\sigma \circ e_1 e_0^{k_1} \dots e_1 e_0^{k_r} &= \sum_{i=1}^{r+1} e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} \sigma e_1 e_0^{k_i} \dots e_1 e_0^{k_r} \\ &- \sum_{i=1}^{r} e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} e_1 \sigma e_0^{k_i} \dots e_1 e_0^{k_r}.\end{aligned}$$

Now consider the terms in this sum arising from a word w appearing in σ. We can assume it occurs with coefficient 1. We obtain terms of two kinds

1. $e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} w e_1 e_0^{k_i} \dots e_1 e_0^{k_r}$
2. $e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} e_1 w^* e_0^{k_i} \dots e_1 e_0^{k_r}$

Note that, for terms of the first type,

$$\deg_{\mathcal{B}}(e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} w e_1 e_0^{k_i} \dots e_1 e_0^{k_r}) = \deg_{\mathcal{B}}(e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} e_1 e_0^{k_i} \dots e_1 e_0^{k_r}) + \deg_{\mathcal{B}}(w)$$

unless $k_{i-1} = 0$. However, in this case, there is a term in the second sum

$$-e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-2}} e_1 w e 1 e_0^{k_i} \dots e_1 e_0^{k_r}$$

that will cancel it out. Similarly, for terms of the second type,

$$\deg_{\mathcal{B}}(e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} e_1 w^* e_0^{k_i} \dots e_1 e_0^{k_r}) = \deg_{\mathcal{B}}(e_1 e_0^{k_1} \dots e_1 e_0^{k_{i-1}} e_1 e_0^{k_i} \dots e_1 e_0^{k_r}) + \deg_{\mathcal{B}}(w)$$

unless $k_i = 0$, in which case there is a term in the first sum that will cancel it out. As such, we can divide the Ihara action into graded pieces.

□

We also recall a short observation due to Charlton [14].

Lemma 2.1.10. *Let $w = w_1 \dots w_n$ be a word in $\{0,1\}^\times$ of length n, with deg$_{\mathcal{B}}(w) = b$. Then $I^{\mathfrak{m}}(w) = 0$ if $b \equiv w + 1$ (mod 2).*

Remark 2.1.11. This provides a natural analogue of the depth parity theorem [10].

Proposition 2.1.12. *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.*

With Proposition 2.2.5, we obtain a similar corollary to the final conclusion of the following corollary.

Corollary 2.1.13. *For a solution to the double shuffle equations mod products $\phi \in \mathfrak{dmr}_0$, of weight N, the depth $d+1 \not\equiv N$ (mod 2) components are uniquely determined by the lower depths. In particular, σ_{2n+1} is uniquely determined in depths 1 and 2.*

Specifically, σ_{2n+1} is uniquely determined in block degree 1 and 2.

2.2 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 algebra $\mathrm{gr}^{\mathcal{B}}\mathcal{A} := \bigoplus_{n=0}^{\infty} \mathcal{B}_n\mathcal{A}/\mathcal{B}_{n-1}\mathcal{A}$. We follow the example of Brown's depth graded multiple zeta values [10].

Remark 2.2.1. In the following it is important to keep in mind that we are identifying $e_i \leftrightarrow \frac{dz}{z-i}$, and, as such, elements of $\mathfrak{g}^{\mathfrak{m}}$ describe relations among iterated integrals, rather than multiple zeta values. As such, our results are 'depth signed' compared to standard notation.

Definition 2.2.2. 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

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

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

Definition 2.2.3. If $\deg_{\mathcal{B}}(e_0 w e_1) = n$, define $\mathrm{I}^{\mathfrak{b}}(0; w; 1)$ to be the image of $\mathrm{I}^{\mathfrak{a}}(0; w; 1)$ in $\mathcal{B}_n\mathcal{A}/\mathcal{B}_{n-1}\mathcal{A}$. Similarly, define $\mathrm{I}^{\mathfrak{bl}}(0; w; 1)$ to be the image of $\mathrm{I}^{\mathfrak{l}}(0; w; 1)$ in $\mathcal{B}_n\mathcal{L}/\mathcal{B}_{n-1}\mathcal{L}$. Define $\zeta^{\mathfrak{b}}$ and $\zeta^{\mathfrak{bl}}$ similarly.

Definition 2.2.4. Fix an embedding of $\{\sigma_3, \sigma_5, \ldots\} \hookrightarrow \mathbb{Q}\langle e_0, e_1\rangle$. 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 $\mathfrak{g}^{\mathfrak{m}}$ 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} and the Ihara bracket.

One of the challenges in studying $\mathfrak{g}^{\mathfrak{m}}$ is that we have an ambiguity in our representation of the generators: σ_{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 2.2.5. *The generators p_{2k+1} of $\mathfrak{bg}$ are canonical, i.e. independent of our choice of embedding of generators $\{\sigma_{2k+1}\} \hookrightarrow \mathbb{Q}\langle e_0, e_1\rangle$.*

Proof. Let σ_{2k+1}, $\sigma'_{2k+1} \in \mathbb{Q}\langle e_0, e_1\rangle$ be two choices of generator for $\mathfrak{g}^{\mathfrak{m}}$ in weight $2k+1$. We must have

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

Proposition 2.1.9 tells us that the Ihara action is compatible with the block filtration, and so

$$\{\mathfrak{g}^{\mathfrak{m}}, \mathfrak{g}^{\mathfrak{m}}\} \subset \mathcal{B}^2\mathfrak{g}^{\mathfrak{m}}$$

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 or $k+1$.

Lemma 2.2.6. *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_0we_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 2.2.7. $\mathfrak{bg}$ *is freely generated by* $\{p_{2k+1}\}_{k\geq 1}$ *as a Lie algebra.*

Proof. We have a bijection between the generators of $\mathfrak{g}^{\mathfrak{m}}$ and of $\mathfrak{bg}$, and Proposition 2.1.9 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 $\mathcal{B}^b\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^{b+1}\mathfrak{g}^{\mathfrak{m}}$. Hence, we have a relation in $\mathfrak{bg}$ if and only if the corresponding sum of terms is 0 in $\mathrm{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$. Indeed, we have an injective Lie algebra homomorphism $\mathfrak{bg} \hookrightarrow \mathrm{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$ induced by the bijection $\{\sigma_{2k+1}\}_{k\geq 1} \leftrightarrow \{p_{2k+1}\}_{k\geq 1}$. Now, as $\mathrm{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$ is dual to $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$, the existence of relations in $\mathfrak{bg}$ implies the existence of additional relations in $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$. To be precise, we must have that

$$\dim\, \mathrm{gr}^{\mathcal{B}}_n\mathcal{L}_N < \dim\, \langle \mathrm{I}^{\mathfrak{l}}(w) | \deg_{\mathcal{B}}(w) = n,\ |w| = N\rangle_{Q}.$$

Then, by the proof of Theorem 7.4 in [9], we know that the right hand side has is spanned by $\{\zeta^{\mathfrak{a}}(k_1,\dots,k_r)\}$, where $k_i \in \{3,2\}$, and $k_i = 3$ exactly n times and $k_1 + \dots + k_r = N$. In particular, it has a basis given by $\zeta^{\mathfrak{a}}(k_1,\dots,k_r)$ 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 $\mathrm{gr}^{\mathcal{B}}_n\mathcal{L}_N$. Thus,

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

which 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, so, no such relation can exist. Thus, we must have that $\mathcal{L} \equiv \mathrm{gr}^{\mathcal{B}}\mathcal{L}$ as they have equal dimensions, and hence, $\mathrm{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}} \equiv \mathfrak{g}^{\mathfrak{m}}$. Thus $\mathrm{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$ is free as a Lie algebra, and hence $\mathfrak{bg}$ is free as a Lie algebra. □

Corollary 2.2.8.

$$\mathfrak{bg} \equiv gr_{\mathcal{L}}\mathfrak{g}^{\mathfrak{m}} \equiv \mathfrak{g}^{\mathfrak{m}}$$

Proof. We have that both $\mathfrak{bg}$ and $\mathfrak{g}^{\mathfrak{m}}$ are non-canonically isomorphic to $\text{Lie}[\sigma_3, \sigma_5, \ldots]$, and hence $\mathfrak{bg} \equiv \mathfrak{g}^{\mathfrak{m}}$. Furthermore, we have $\mathfrak{bg} \hookrightarrow \text{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$, and the dimension of the weight N piece of $\text{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$ is equal to the dimension of the weight N piece of $\mathfrak{g}^{\mathfrak{m}} \equiv \text{Lie}[\sigma_3, \sigma_5, \ldots] \equiv \mathfrak{bg}$, and hence we must have $\mathfrak{bg} \equiv \text{gr}_{\mathcal{B}}\mathfrak{g}^{\mathfrak{m}}$. □

Remark 2.2.9. While both Brown's $\mathfrak{dg}$ and our $\mathfrak{bg}$ have canonical generators, Theorem 2.2.7 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 [37], and this has been further explored by Baumard and Schneps [4]. 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.

2.3 Polynomial representations

We now reframe this Lie algebra in terms of commutative polynomials, similarly to Brown [12][13] and Écalle [21], 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 [14]. In doing so, he establishes a bijection

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

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

Example 2.3.1.

$$e_0e_1e_0e_0e_1e_0e_1e_1 \mapsto (0; 3, 4, 1),$$

$$e_1e_1e_0e_1e_0e_1e_1e_0e_0 \mapsto (1; 1, 5, 2, 1)$$

Definition 2.3.2. Define $\mathrm{I}^{\mathfrak{m}}(l_1,\ldots,l_n) := \mathrm{I}^{\mathfrak{m}}(0;a_1,\ldots,a_k;a_{k+1})$, where the a_i are determined by $\mathrm{bl}(e_0e_{a_1}\ldots e_{a_{k+1}}) = (0;l_1,\ldots,l_n)$.

We can use the map bl to define an injection of vector spaces by

$$\begin{aligned} \pi_{\mathrm{bl}} : \mathbb{Q}\langle e_0,e_1\rangle \setminus \{\mathbb{Q}\cdot 1\} &\to \bigoplus_{n=1}^{\infty} \mathbb{Q}[x_1,\ldots,x_n] \\ w &\mapsto x_1^{l_1}\ldots x_n^{l_n} \end{aligned} \tag{2.3.1}$$

where $\mathrm{bl}(e_0we_1) = (0;l_1,\ldots,l_n)$. The image of this injection is given by

$$\bigoplus_{n=1}^{\infty} x_1\ldots x_n\mathbb{Q}[x_1,\ldots,x_n]^o$$

where $\mathbb{Q}[x_1,\ldots,x_n]$ consists of polynomials of odd degree. This parity requirement is a consequence of Lemma 2.1.10.

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 injection.

Proposition 2.3.3. *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

$$q_{2k+1}(x_1,x_2) = \sum_{i=1}^{k}\left[\binom{2k}{2i} - \left(1-\frac{1}{2^{2k}}\right)\binom{2k}{2k+1-2i}\right]x_1^{2i+1}x_2^{2k+2-2i} - x_1x_2^{2k+2}$$

and σ_{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 σ_{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

$$q_{2k+1} = \sum_{i=0}^{k} c_i(e_1e_0)^ie_0(e_1e_0)^{k-i},$$

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 [9].

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 [42],

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

Brown then shows in [9] Theorem 4.3 that this lifts to an identity among motivic multiple zeta values. Considered modulo $\zeta^{\mathfrak{m}}(2)$, we find

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

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

□

Computing these sums explicitly, we obtain the following theorem.

Theorem 2.3.4.

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

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

Corollary 2.3.5. *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*

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

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 $p(x_1,x_2)=x_1x_2(x_1-x_2)r(x_1,x_2)$. 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 $(2k+3)-3=2k$

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

which is to say

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

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 $\mathfrak{g}^{\mathfrak{m}}$ 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 2.3.6. *For (depth-signed) elements of the motivic Lie algebra, the Ihara action* *is given at the level of block-polynomials for each block homogeneous piece by*

$$\begin{aligned}(f \circ g)(x_1, \ldots, x_{m+n-1}) = (-1)^{(m+1)(n+1)} \sum_{i=1}^{n} & \frac{f(x_i, x_{i+1}, \ldots, x_{i+m-1})}{x_i - x_{i+m-1}} \\ & \times \left(\frac{1}{x_i} g(x_1, \ldots, x_{i-1}, x_i, x_{i+m}, \ldots, x_{m+n-1}) \right. \\ & \left. - \frac{1}{x_{i+m-1}} g(x_1, \ldots, x_{i-1}, x_{i+m-1}, \ldots, x_{m+n-1}) \right). \end{aligned} \tag{2.3.2}$$

2.4 Relations arising in the polynomial representation

We find several relations arising naturally in the polynomial representation which are preserved by the Ihara action, and dual to relations in $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$. We prove these by induction on the block degree. We illustrate the method by reproving that the duality arising from the symmetry $0 \leftrightarrow 1$ of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ holds. While this is not a new result, it serves to demonstrate the approach in a case where all computations remain simple.

Proposition 2.4.1. *For all* $f(x_1, \ldots, x_n) \in \mathfrak{bg}$,

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

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

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

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

and hence, the duality relation is preserved by the Ihara bracket. □

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. We will instead show that a more general relation holds, of which cyclic insertion is a corollary. These are the 'block shuffle' relations.

Definition 2.4.2. For any $1 \le r \le n$, define the shuffle set

$$\mathrm{Sh}_{n,r} = \{\sigma \in \mathcal{S}_n | \sigma^{-1}(1) < \ldots < \sigma^{-1}(r); \sigma^{-1}(r+1) < \ldots < \sigma^{-1}(n)\}.$$

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

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

Theorem 2.4.3. *For any $f(x_1,\ldots,x_n) \in \mathfrak{bg}$, and any $1 \le r < n$, we have*

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

Proof. For p_{2k+1}, this is equivalent to $p(x_1,x_2)+p(x_2,x_1)=0$, given by Proposition 2.4.1. Then, as the Ihara action is associative, it in fact suffices to show that

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

for all $f = p_{2k+1}(x_1,x_2)$, $g(x_1,\ldots,x_n) \in \mathfrak{bg}$.

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

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

This sum splits as follows

$$\sum_{\sigma\in \mathrm{Sh}_{n+1,r}} \sum_{i=1}^{r-1} \frac{f\big(x_{\sigma(i)}, x_{\sigma(i+1)}\big)}{x_{\sigma(i)} - x_{\sigma(i+1)}} \times$$
$$\left(\frac{g\big(x_{\sigma(1)}, \ldots, x_{\sigma(i)}, x_{\sigma(i+2)}, \ldots, x_{\sigma(n+1)}\big)}{x_{\sigma(i)}} - \frac{g\big(x_{\sigma(1)}, \ldots, x_{\sigma(i-1)}, x_{\sigma(i+1)}, \ldots, x_{\sigma(n+1)}\big)}{x_{\sigma(i+1)}} \right)$$
$$+ \sum_{\sigma\in \mathrm{Sh}_{n+1,r}} \sum_{i=r+1}^{n} \frac{f\big(x_{\sigma(i)}, x_{\sigma(i+1)}\big)}{x_{\sigma(i)} - x_{\sigma(i+1)}} \times$$
$$\left(\frac{g\big(x_{\sigma(1)}, \ldots, x_{\sigma(i)}, x_{\sigma(i+2)}, \ldots, x_{\sigma(n+1)}\big)}{x_{\sigma(i)}} - \frac{g\big(x_{\sigma(1)}, \ldots, x_{\sigma(i-1)}, x_{\sigma(i+1)}, \ldots, x_{\sigma(n+1)}\big)}{x_{\sigma(i+1)}} \right)$$
$$+ \sum_{\substack{\sigma\in \mathrm{Sh}_{n+1,r} \\ \text{such that} \\ \{\sigma(r),\sigma(r+1)\}\neq\{r,r+1\}}} \frac{f\big(x_{\sigma(r)}, x_{\sigma(r+1)}\big)}{x_{\sigma(r)} - x_{\sigma(r+1)}} \times$$
$$\left(\frac{g\big(x_{\sigma(1)}, \ldots, x_{\sigma(r)}, x_{\sigma(r+2)}, \ldots, x_{\sigma(n+1)}\big)}{x_{\sigma(r)}} - \frac{g\big(x_{\sigma(1)}, \ldots, x_{\sigma(r-1)}, x_{\sigma(r+1)}, \ldots, x_{\sigma(n+1)}\big)}{x_{\sigma(r+1)}} \right).$$

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

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

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

1. $l \le r$,
2. $k \ge r+1$,
3. $k < r < r+1 < l$,
4. $k = r = l-1$.

In the first case, both A and 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

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

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

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

Then, this is a sum over the set of permutations

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

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

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

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

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

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

All of these must be empty due to the order preserving property of shuffle permutations. Thus,

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

$\square$

Corollary 2.4.4. *For any finite sequence of integers $l_1, \dots, l_n$, and any $1 \leq r < n$, we have*

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

when considered modulo products.

Proof. Using Theorem 2.2.7, we can consider $\mathfrak{bg}$ as the dual Lie algebra to the graded Lie coalgebra of indecomposables $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$, and hence, relations among the coefficients of elements of $\mathfrak{bg}$ induce relations among elements of $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$. Specifically, we define a $\mathbb{Q}$-linear pairing

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

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

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

$\square$

Corollary 2.4.5 (Block graded cyclic insertion)**.** *The cyclic sum*

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

Proof. It suffices to show that

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

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

Suppose $f \in \mathfrak{bg}$. Then, Theorem 2.4.3 implies that the image of f under the following vector space isomorphism

$$\begin{gathered} \bigoplus_{n=0}^{\infty} \mathbb{Q}[x_1, \dots, x_n] \xrightarrow{\sim} \mathbb{Q}\langle z_1, z_2, z_3, \dots \rangle \\ x_1^{i_1} x_2^{i_2} \dots x_n^{i_n} \mapsto z_{i_1} z_{i_2} \dots z_{i_n} \end{gathered} \tag{2.4.1}$$

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

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

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

Note, 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 $\sigma \in \mathrm{C}_n$ 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 $\mathrm{Lie}[z_1, z_2, \dots]$ is zero, and hence

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

□

Remark 2.4.6. As in this proof, it can be useful to consider $\mathfrak{bg}$ as a subspace of the Hopf $\mathbb{Q}\langle z_1, z_2, z_3, \dots \rangle$, with the standard concatenation product, and a coproduct given by $\Delta z_i = z_i \otimes 1 + 1 \otimes z_i$. For example, Theorem 2.4.3 implies elements of $\mathfrak{bg}$ are primitive for this coproduct, we immediately obtain Proposition 2.4.1 as a corollary, by considering the antipode map, i.e. the antihomomorphism $z_i \mapsto -z_i$. This is an idea explored further in Section 2.11.

2.5 Shuffle Regularisation

The double shuffle relations among iterated integrals are not, in general, compatible with the block filtration. However, the regularisation relation obtained by shuffling with an element of weight 1, does respect the block filtration.

Theorem 2.5.1. *Let* $\pi_1 : \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}e_0 \oplus \mathbb{Q}e_1$ *denote the projection map onto weight 1 , and let* $\Delta : \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle e_0, e_1\rangle \otimes \mathbb{Q}\langle e_0, e_1\rangle$ *be the coproduct defined by* $\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i$*. The map* $\Delta_1 := (\pi_1 \otimes id)\Delta$ *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 $i \in \{0, 1\}$, where $\bar{w}$ is obtained from w by omitting a letter. The left hand side is of block degree 1. The right hand side is of higher block degree, if the omitted letter was internal to a block, and of block degree 1 lower than w, if the omitted letter was at the beginning or end of a block. □

Thus, we can take the associated graded map of Δ_1.

Corollary 2.5.2. $gr_{\mathcal{B}}(\Delta_1)(\mathfrak{bg}) = 0$.

Proof. This follows from the work of Brown [9] and Racinet [38], as any element $\psi \in \mathfrak{g}^{\mathfrak{m}}$ satisfies $\Delta(\psi) = 0$. □

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

Example 2.5.3. For $f(x_1, x_2) \in \mathfrak{bg}$ and $g(x_1, x_2, x_3) \in \mathfrak{bg}$, we have

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

In order to better describe elements of $\mathfrak{bg}$, we use the following lemma to transform our polynomial representation.

Lemma 2.5.4. *For $f(x_1, x_2, \ldots, x_n) \in \mathfrak{bg}$, we can write*

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

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

Proof. We induct on the number of variables. For $n = 2$, this follows from Theorem 2.3.4. Now, suppose this factorisation holds for $f(x_1, x_2)$, $g(x_1, \ldots, x_n) \in \mathfrak{bg}$. We have

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

Applying our induction hypothesis, we find

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

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

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 $x_1 \dots x_{n+1}(x_1 - x_{n+1})$. This is clear, so we are done.

□

Definition 2.5.5. 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 2.5.6. 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 $n-1$.

2.6 The dihedral action

As an immediate corollary to Proposition 2.4.1 we obtain:

Lemma 2.6.1. *For all* $r(x_1, \ldots, x_n) \in \mathfrak{rdg}$*,*

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

Definition 2.6.2. We define a Lie algebra structure on $\mathfrak{rdg}$ via the Lie bracket

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

for $r_1(x_1, \ldots, x_m) = \frac{f_1(x_1,\ldots,x_m)}{x_1\ldots x_m(x_1-x_m)}, r_2(x_1, \ldots, x_n) = \frac{f_2(x_1,\ldots,x_n)}{x_1\ldots x_n(x_1-x_n)} \in \mathfrak{rdg}$. 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 2.6.3. *For* $r(x_1, x_2),\ q(x_1, \ldots, x_{n-1}) \in \mathfrak{rdg}$*, the reduced Ihara bracket is given by*

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

where we consider indices modulo n*.*

Corollary 2.6.4.

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

for $r(x_1, \ldots, x_n) \in \mathfrak{rdg}$*.*

Proof. This follows from a simple induction argument, using Lemma 2.6.1 as our base case, and the natural cyclic symmetry in Proposition 2.6.3. □

Remark 2.6.5. Corollary 2.4.5 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 2.6.6. *For* $r(x_1, \ldots, x_m), q(x_1, \ldots, x_n) \in \mathfrak{rdg}$*, the reduced Ihara bracket is given* *by*

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

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

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

2.7 A differential relation

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

Definition 2.7.1. For $n \geq 2$, define the differential operator

$$\mathrm{D}_n : \mathbb{Q}[x_1,\dots,x_n] \to \mathbb{Q}[x_1,\dots,x_n]$$

by

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

Theorem 2.7.2.

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

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

Proof. We induct on n. For $n=2$, this follows from Corollary 2.3.5. Suppose this holds for $q(x_1,\dots,x_n) \in \mathfrak{rbg}$.

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 $\mathrm{D}_n = \prod_{M\in I_n} L_M$, and thus we have, for $r(x_1,x_2), q(x_1,\dots,x_n) \in \mathfrak{rbg}$,

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

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

Next 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 $M[i,i+1] = \left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right)$ for all $M\in S$, or $M[i,i+1] = \left(\begin{smallmatrix}1&-1\\-1&1\end{smallmatrix}\right)$ for all $M\in S$. In the first case, we must have all $M\in I_{n+1}$ with $M[i,i+1] = \left(\begin{smallmatrix}1&-1\\-1&1\end{smallmatrix}\right)$ contained in $I_{n+1}\setminus S$. The second case is similar. 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

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

Thus $D_{n+1}\{r,q\}$=0. □

Remark 2.7.3. By direct computation, one can show that, in sufficiently high degree, $r(x_1,\dots,x_n)\in \ker\mathrm{D}_n$ is equivalent to $r(x_1,\dots,x_n)\in\sum_{M\in I_n}\ker L_M$. As an illustration, consider solving the inhomogeneous equation

$$(Lf)(x_1,x_2,x_3) = (\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3})(f)(x_1,x_2,x_3) = (x_1+x_2)^a(x_2-x_3)^b$$

The right hand side is an element of the kernel of $R = (\frac{\partial}{\partial x_1} - \frac{\partial}{\partial x_2} - \frac{\partial}{\partial x_3})$. Making a change of variables to $u = x_1 + x_2$, $v = x_2 - x_3$, $w = x_1 - x_2$, we obtain that

$$2\frac{\partial f}{\partial u} = u^a v^b$$

which clearly only has solutions of the form

$$f(u,v,w) = \frac{1}{2a+2}u^{a+1}v^b + Cv^s w^t = \frac{1}{2a+2}(x_1+x_2)^{a+1}(x_2-x_3)^b + C(x_1-x_2)^t(x_2-x_3)^s.$$

This is an element of $\ker L + \ker R$. By similar changes of variables, this argument generalises.

This alternative condition clearly holds for $n = 2$, and can easily be shown to be preserved by the Ihara bracket. Hence, we can equivalently state Theorem 2.7.2 as the following:

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

Remark 2.7.4. Corollary 2.3.5 shows that in block degree 1, $\mathfrak{bg}$ is isomorphic as a vector space to the bigraded vector space of homogeneous polynomials satisfying the *block relations*:

(1): $f(x_1 \ldots x_k ⧢ x_{k+1} \ldots x_n) = 0$ for any $1 \le k < n$,

(2): $f(x_1, \ldots, x_n) = x_1 \ldots x_n (x_1 - x_n) r(x_1, \ldots, x_n)$, $r(x_1, \ldots, x_n) \in \mathbb{Q}[x_1, \ldots, x_n]$,

(3): $\mathrm{D}_n r = 0$,

(4): $r(x_1, \ldots, x_n) = r(x_2, \ldots, x_n, x_1) = (-1)^n r(x_n, \ldots, x_1)$,

(5): f satisfies shuffle regularisation, as in Example 2.5.3.

Note also that, as all these properties are preserved by the Ihara bracket, $\mathfrak{bg}$ 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.

2.8 Further results in block degree two

While we can uniquely described elements of $\mathfrak{bg}_1$ as solutions to a set of equations, in block degree two we can only bound the dimension above by something growing linearly in weight using the same relations. We can, however, describe where the "missing" relations lie. Let $r(x_1, x_2, x_3) \in \mathfrak{rbg}_2$. Then we have that

$$r(x_1, x_2, x_3) = r(x_2, x_3, x_1) = -r(x_3, x_2, x_1),$$

$$\frac{\partial^4 r}{\partial x_1^4} + \frac{\partial^4 r}{\partial x_2^4} + \frac{\partial^4 r}{\partial x_3^4} - 2\frac{\partial^4 r}{\partial x_1^2 \partial x_2^2} - 2\frac{\partial^4 r}{\partial x_2^2 \partial x_3^2} - 2\frac{\partial^4 r}{\partial x_3^2 \partial x_1^2} = 0,$$

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:

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

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

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

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

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

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 $r(x_1, x_2, x_3) \in \mathfrak{rbg}_2$ such that $q_o(x_1, x_2, x_3) = r_o(x_1, x_2, x_3)$. Equivalently, we claim the following.

Proposition 2.8.1. *Let $V_o^{2n} \subset \mathbb{Q}[x_1, x_2, x_3]$ be the space of homogeneous polynomials of* *degree $2n$, satisfying*

$$\textit{Equation (1): } q(x_1,x_2,x_3) = q(x_2,x_3,x_1) = -q(x_3,x_2,x_1),$$

$$\textit{Equation (2): } \frac{1}{2}\left(q(0,y,z) - q(0,y,-z)\right) = q(-y,y,z) - q(y,-z,z),$$

$$\textit{Equation (3): } \frac{\partial^4 q}{\partial x_1^4} + \frac{\partial^4 q}{\partial x_2^4} + \frac{\partial^4 q}{\partial x_3^4} - 2\frac{\partial^4 q}{\partial x_1^2 \partial x_2^2} - 2\frac{\partial^4 q}{\partial x_2^2 \partial x_3^2} - 2\frac{\partial^4 q}{\partial x_3^2 \partial x_1^2} = 0,$$

$$\textit{Equation (4): } q_e(x_1,x_2,x_3) = 0,$$

and let $d_{2,2n}$ be the dimension of the degree $2n$ piece of $\mathfrak{rbg}_2$, i.e. the dimension of the weight $2n+2$ part of $\mathfrak{bg}_2$. 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 $k,l \geq 1$. This is precisely the number of positive integer solutions to $k+l=n$ with $1 \leq k < l$. Thus $d_{2,2n} = \lfloor \frac{n-1}{2} \rfloor$.

Next, Equation (3) implies

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

Define $q_\star(x_1,x_2,x_3) := \frac{1}{4}\left(q(x_1,x_2,x_3) - q(-x_1,x_2,x_3) - q(x_1,x_2,-x_3) + q(-x_1,x_2,-x_3)\right)$; this the part of q that is odd in x_1 and x_3 and even in x_2. We can write

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

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 $q_\star(x_1,x_2,x_3)$ 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

$$q(x_1,x_2,x_3) = q_\star(x_1,x_2,x_3) + q_\star(x_2,x_3,x_1) + q_\star(x_3,x_1,x_3).$$

Thus, q is uniquely determined by $q_\star$. We currently have $n-1$ free variables in $q_\star$, 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 $q_\star(x_1, x_2, x_3)$, we find that we must have

$$q_\star(z, 0, y) = 2q_\star(z, y, y) - 2q_\star(y, z, z).$$

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

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

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

$$\rho_{l,k} \equiv 0 \text{ mod } 2,$$

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

As such, we can quantify the number of "missing" relations by computing the dimension of totally even polynomials satisfying the defining relations.

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

Denote by V_e^{2n} the vector space of such polynomials, homogeneous of degree $2n$.

Proposition 2.8.2.

$$dim\ V_e^{2n} = \lfloor \frac{n}{3} \rfloor$$

Proof. We first note that, if

$$\frac{\partial^4 q}{\partial x_1^4}+\frac{\partial^4 q}{\partial x_2^4}+\frac{\partial^4 q}{\partial x_3^4}-2\frac{\partial^4 q}{\partial x_1^2\partial x_2^2}-2\frac{\partial^4 q}{\partial x_2^2\partial x_3^2}-2\frac{\partial^4 q}{\partial x_3^2\partial x_1^2}=0,$$

and $q(x_1,x_2,x_3)$ is even in all its variables, we can write

$$\begin{aligned} q(x_1,x_2,x_3) = \sum_{\substack{i+j=2n\\ i,j\geq 0}} \epsilon_{i,j}\big((x_1-x_2)^i(x_2-x_3)^j+(-1)^i(x_1+x_2)^i(x_2-x_3)^j \\ +(x_1-x_2)^i(x_2+x_3)^j+(-1)^i(x_1+x_2)^i(x_2+x_3)^j\big)\,. \end{aligned}$$

Indeed, the set

$$\mathcal{Q} := \{(x_1-x_2)^i(x_2-x_3)^j+(-1)^i(x_1+x_2)^i(x_2-x_3)^j+(x_1-x_2)^i(x_2+x_3)^j+(-1)^i(x_1+x_2)^i(x_2+x_3)^j\}_{i+j=2n}$$

forms a basis for the space of totally even solutions of

$$\frac{\partial^4 q}{\partial x_1^4}+\frac{\partial^4 q}{\partial x_2^4}+\frac{\partial^4 q}{\partial x_3^4}-2\frac{\partial^4 q}{\partial x_1^2\partial x_2^2}-2\frac{\partial^4 q}{\partial x_2^2\partial x_3^2}-2\frac{\partial^4 q}{\partial x_3^2\partial x_1^2}=0.$$

Then, as $\frac{1}{2}\left(q(0,y,z)-q(0,y,-z)\right)=q(-y,y,z)-q(y,-z,z)$ holds trivially for any totally even polynomial satisfying the symmetry conditions, it is sufficient to compute the dimension of the subspace of skew-symmetric polynomials spanned by $\mathcal{Q}$. This is a simple representation theoretic argument: we consider $Span(\mathcal{Q})$ as a representation of the symmetric group S_3 via the standard polynomial representation, and compute the dimension of the sign representation within this. In particular, representation theory says that

$$\begin{aligned} \dim V_e^{2n} &= \frac{1}{6}\left[\mathrm{Tr}(id)-3\mathrm{Tr}((13))+2\mathrm{Tr}((123))\right] \\ &= \frac{1}{6}\left[2n+1-3\mathrm{Tr}((13))+2\mathrm{Tr}((123))\right]. \end{aligned}$$

Note that the vector spaces generated by $\{(x_1-x_2)^i(x_2-x_3)^j\}_{i+j=2n}$ and $\{(x_1+x_2)^i(x_2-x_3)^j,\ (x_1-x_2)^i(x_2+x_3)^j,\ (x_1+x_2)^i(x_2+x_3)^j\}_{i+j=2n}$ are invariant under the action of S_3, and so it is sufficient to consider the trace of the action restricted to $\{(x_1-x_2)^i(x_2-x_3)^j\}_{i+j=2n}$.

Clearly, the trace of (13) is 1, as the only diagonal entry corresponds to $(x_1-x_2)^n(x_2-$

$x_3)^n \mapsto (x_3 - x_2)^n(x_2 - x_1)^n$. Now, computing the trace of (123), we find that it is given by

$$\sum_{i=0}^{2n} (-1)^i \binom{2n-i}{i}.$$

To compute this, we consider the generating series

$$\begin{aligned}\sum_{n\geq 0}\sum_{i=0}^{n} \binom{n-i}{i} x^i y^n &= \sum_{k\geq 0}\sum_{i\geq 0} \binom{k}{i} (xy)^i y^k \\ &= \sum_{k\geq 0} (1+xy)^k y^k \\ &= \frac{1}{1-y-xy^2}.\end{aligned}$$

Setting $x = -1$, we obtain

$$\begin{aligned}\sum_{n\geq 0}\sum_{i=0}^{n} (-1)^i \binom{n-i}{i} (-y)^n &= \frac{1}{1+y+y^2} \\ &= \frac{1-y}{1-y^3} \\ &= \sum_{m\geq 0} y^{3m} - y^{3m+1}.\end{aligned}$$

Thus,

$$\sum_{i=0}^{2n} (-1)^i \binom{2n-i}{i} = \begin{cases} 1 & \text{if } 2n \equiv 0 \bmod 6 \\ -1 & \text{if } 2n \equiv 4 \bmod 6 \\ 0 & \text{if } 2n \equiv 2 \bmod 6 \end{cases}$$

Hence

$$\dim V_e = \frac{1}{6}\left(2n + 1 - 3 + 2x\right),$$

where x is determined by $2n$ mod 6. A quick consideration of each case shows we obtain $\lfloor \frac{2n}{6} \rfloor = \lfloor \frac{n}{3} \rfloor$.

$\square$

While we have been unable to describe $\mathfrak{rdg}_2$ completely in terms of equations, we can provide a complete characterisation. In particular, we show that you can recover $r_e(x_1, x_2, x_3)$ from $r_{oeo}(x_1, 0, x_3)$. We first claim that, in order to obtain a vector space of the correct dimension, it is sufficient to determine the coefficient of $x_1^{2a+3}x_2x_3^{2b+2}$ for all $a, b \geq 0$ in $f(x_1, x_2, x_3) \in \mathfrak{bg}$. This is equivalent to somehow specifying the value of $\zeta^{\mathfrak{bl}}(\{2\}^a, 4, \{2\}^b)$ relative to our normalisation of the generators σ_{2k+1}. We will expand on what we mean by this precisely in a moment. First we will show that the coefficients of $x_1^{2a+3}x_2x_3^{2b+2}$ provide sufficient information.

Let $f(x_1, x_2, x_3) \in x_1x_2x_3(x_1 - x_3)\mathbb{Q}[x_1, x_2, x_3]$ be homogeneous of degree $2n + 4$, and let $r(x_1, x_2, x_3) = \frac{f(x_1,x_2,x_3)}{x_1x_2x_3(x_1-x_3)}$ be it's reduced form. Let $\alpha_{i,j,k}$ be the coefficient of $x_1^i x_2^j x_3^k$ in $r(x_1, x_2, x_3)$. Now suppose $r(x_1, x_2, x_3)$ satisfies the first three conditions in Proposition 2.8.1. Then, as described in Propositions 2.8.1 and 2.8.2, the 'odd' part of $r(x_1, x_2, x_3)$ lies in a vector space of dimension $\dim \mathfrak{rbg}_{2,2n}$, the degree $2n$ piece of $\mathfrak{rbg}_2$, while the totally even part lies in a vector space of dimension $\lfloor \frac{n}{3} \rfloor$. We want to impose additional relations so that $r(x_1, x_2, x_3)$ lies in a vector space of dimension exactly $\dim \mathfrak{rbg}_{2,2n}$. It is therefore sufficient to impose relations with which we can calculate the totally even part from the 'odd' part.

Lemma 2.8.3. *Let $r(x_1, x_2, x_3)$ be as above, and suppose $r(x_1, x_2, x_3) - r_e(x_1, x_2, x_3)$ is fixed. Suppose also that the coefficient of $x_1^{2a+3}x_2x_3^{2n-2a}$ in $x_1x_2x_3(x_1 - x_3)r(x_1, x_2, x_3)$ is fixed for each a: call it c_a. Then $r_e(x_1, x_2, x_3)$ is uniquely determined.*

Proof. The coefficients c_a are related to the coefficients of $r(x_1, x_2, x_3)$ by

$$c_a = \alpha_{2a+1,0,2n-2a-1} - \alpha_{2a+2,0,2n-2a-2}$$

and hence

$$\alpha_{2a+2,0,2n-2a-2} = \alpha_{2a+1,0,2n-2a-1} - c_a.$$

Thus the coefficients $\alpha_{2k,0,2m}$ are determined. This, in fact, determines all the coefficients $\alpha_{2k,2l,2m}$. Recall that $r_e(x_1, x_2, x_3)$ satisfies

$$\frac{\partial^4 r_e}{\partial x_1^4} + \frac{\partial^4 r_e}{\partial x_2^4} + \frac{\partial^4 r_e}{\partial x_3^4} - 2\frac{\partial^4 r_e}{\partial x_1^2 \partial x_2^2} - 2\frac{\partial^4 r_e}{\partial x_2^2 \partial x_3^2} - 2\frac{\partial^4 r_e}{\partial x_3^2 \partial x_1^2} = 0$$

and hence is of the form

$$r_e(x_1,x_2,x_3) = \sum_{\substack{i+j=2n\\ i,j\geq 0}} \epsilon_{i,j}\left((x_1-x_2)^i(x_2-x_3)^j + (-1)^i(x_1+x_2)^i(x_2-x_3)^j\right.$$

$$\left. +(x_1-x_2)^i(x_2+x_3)^j + (-1)^i(x_1+x_2)^i(x_2+x_3)^j\right).$$

Setting $x_2 = 0$, we get that

$$\sum_{\substack{s+t=n\\ s,t\geq 0}} \alpha_{2s,0,2t}x_1^{2s}x_3^{2t} = \sum_{\substack{i+j=2n\\ i,j\geq 0}} 2\epsilon_{i,j}\left((-1)^i x_1^i x_3^j + x_1^i x_3^j\right)$$

and hence $\epsilon_{2s,2t} = \frac{1}{4}\alpha_{2s,0,2t}$. Then, as in the proof of Proposition 2.8.2, we note that the vector spaces generated by

$$\{(x_1-x_2)^i(x_2-x_3)^j\}_{i+j=2n}$$

and

$$\{(x_1+x_2)^i(x_2-x_3)^j,\ (x_1-x_2)^i(x_2+x_3)^j,\ (x_1+x_2)^i(x_2+x_3)^j\}_{i+j=2n}$$

are invariant under the action of S_3, and so $r_e(x_1,x_2,x_3) = r_e(x_2,x_3,x_1)$ implies that

$$\sum_{\substack{i+j=2n\\ i,j\geq 0}} \epsilon_{i,j}\left((x_1-x_2)^i(x_2-x_3)^j\right) = \sum_{\substack{i+j=2n\\ i,j\geq 0}} \epsilon_{i,j}\left((-1)^i(x_2-x_3)^i(x_1-x_3)^j\right).$$

Expanding $(x_1-x_3)^j = (x_1-x_2+x_2-x_3)^j$ and comparing coefficients of $(x_1-x_2)^s(x_2-x_3)^t$, we obtain that

$$\epsilon_{s,t} = \sum_{\substack{i+j=2n\\ i,j\geq 0}} (-1)^i\binom{j}{s}\epsilon_{i,j}.$$

In particular, this implies

$$\epsilon_{2s+1,2t-1} = \frac{1}{2s+1}\left(2\epsilon_{2s,2t} - \sum_{\substack{i+j=2n\\ i\geq 0, j\geq 2s+2}} (-1)^i\binom{j}{2s}\epsilon_{i,j}\right)$$

which recursively determines $\epsilon_{2s+1,2t-1}$ in terms of $\epsilon_{2i,2j}$. Thus, $r_e(x_1,x_2,x_3)$ is uniquely determined by $\alpha_{2s,0,2t}$, and the result follows. □

To determine the coefficients of $x_1^{2a+3}x_2x_3^{2n-2}$, we utilise the motivic machinery introduced by Brown [9]. Brown defines a non-canonical Hopf algebra isomorphism $\Phi : \mathcal{A} \to \mathbb{Q}\langle f_3, f_5, \ldots\rangle$ from the space of de Rham multiple zeta values with the motivic coproduct to $\mathbb{Q}\langle f_3, f_5, f_7, \ldots\rangle$ equipped with the shuffle product and deconcatenation coproduct given by

$$\Delta(f_{i_1} \ldots f_{i_n}) = \sum_{k=0}^{n} f_{i_1} \ldots f_{i_k} \otimes f_{i_{k+1}} \ldots f_{i_n}.$$

This isomorphism is determined by a choice of elements mapping onto the set $\{f_{2k+1}\}_{k\geq 1}$. In this, we deviate slightly from Brown's approach. Instead of choosing $\Phi(\zeta^{\mathfrak{a}}(2k+1)) = f_{2k+1}$, we will rescale so that $\Phi(\zeta^{\mathfrak{a}}(2k+1)) = a_{2k+1}^{-1} f_{2k+1}$, where a_{2k+1} is the coefficient of $e_1 e_0^{2k}$ in σ_{2k+1}.

Note that the block filtration, which by Corollary 2.1.8 agrees with coradical filtration, induces a filtration on $\mathbb{Q}\langle f_3, f_5, \ldots\rangle$ given by

$$\mathcal{B}_n\mathbb{Q}\langle f_3, f_5, \ldots\rangle = \langle f_{i_1} f_{i_2} \ldots f_{i_k} \ : \ k \leq n\rangle_{\mathbb{Q}}.$$

We can define a pairing $\langle \cdot, \cdot\rangle : \mathcal{L} \otimes \mathfrak{g}^{\mathfrak{m}} \to \mathbb{Q}$ where $\langle \mathrm{I}^{\mathfrak{l}}(0; w; 1), \sigma\rangle$ is the coefficient of w in σ. Via Φ, this induces a pairing

$$\mathbb{Q}\langle f_3, f_5, \ldots\rangle / \mathbb{Q}\langle f_3, f_5, \ldots\rangle^{ш 2} \otimes \mathfrak{g}^{\mathfrak{m}} \to \mathbb{Q}$$

In particular, we have $\langle f_{2k+1}, \sigma_{2l+1}\rangle = \delta_{k,l}$.

The (induced) motivic coproduct on $\mathcal{L}$ is dual to the Ihara action on $\mathbb{Q}\langle e_0, e_1\rangle$, and we therefore have that

$$\langle\{\sigma_{2k+1}, \sigma_{2l+1}\}, \mathrm{I}^{\mathfrak{l}}(0; w; 1)\rangle = \langle\sigma_{2k+1} \otimes \sigma_{2l+1}, \Delta(\mathrm{I}^{\mathfrak{l}}(0; w; 1)\rangle - \langle\sigma_{2l+1} \otimes \sigma_{2k+1}, \Delta(\mathrm{I}^{\mathfrak{l}}(0; w; 1))\rangle.$$

Since Δ acts by deconcatenation, this extracts the coefficients of $f_{2k+1}f_{2l+1}$ and $f_{2l+1}f_{2k+1}$ in $\Phi(\mathrm{I}^{\mathfrak{l}}(0; w; 1))$. Denoting by $\pi_{2k+1,2l+1}(w)$ the coefficient of $f_{2k+1}f_{2l+1}$ in $\Phi(\mathrm{I}^{\mathfrak{l}}(0; w; 1))$, we have shown the following lemma.

Lemma 2.8.4. *The coefficient of w in $\{\sigma_{2k+1}, \sigma_{2l+1}\}$ is given by*

$$\pi_{2k+1,2l+1}(w) - \pi_{2l+1,2k+1}(w).$$

In particular, we can consider the block degree 2 part to obtain the following corollary.

Corollary 2.8.5. *Let $c^{2s+1}_{i,j}$ be the coefficient of $x_1^i x_2^j$ in $p_{2s+1}(x_1, x_2)$. Then the coefficient of $x_1^{2a+3}x_2x_3^{2n-2a}$ in $\{p_{2n-2k+1}, p_{2k+1}\}$ is given by*

$$\begin{aligned} &c^{2k+1}_{1,2k+2}c^{2n-2k+1}_{2a+3,2n-2a-2k}\mathbb{1}_{n\geq a+k+1} - c^{2k+1}_{1,2k+2}c^{2n-2k+1}_{2a-2k+3,2n-2a}\mathbb{1}_{a\geq k}\\ -&c^{2n-2k+1}_{1,2n-2k+2}c^{2k+1}_{2a+3,2k-2a}\mathbb{1}_{k\geq a+1} + c^{2n-2k+1}_{1,2n-2k+2}c^{2k+1}_{2a+2k-2n+3,2n-2a}\mathbb{1}_{a+k\geq n}.\end{aligned}$$

In particular, normalising $\{p_{2s+1}\}_{s\geq 1}$ so that $c^{2s+1}_{1,2s+2} = -1$ for all s, this is given by

$$\begin{aligned} &\left[\binom{2n-2k}{2a-2k+2} - (1 - \frac{1}{2^{2n-2k}})\binom{2n-2k}{2a-2k+1}\right]\mathbb{1}_{a\geq k}\\ +&\left[\binom{2k}{2a+2} - (1 - \frac{1}{2^{2k}})\binom{2k}{2a+1}\right]\mathbb{1}_{k\geq a+1}\\ -&\left[\binom{2n-2k}{2a+2} - (1 - \frac{1}{2^{2n-2k}})\binom{2n-2k}{2a+1}\right]\mathbb{1}_{n\geq a+k+1}\\ -&\left[\binom{2k}{2a+2k-2n+2} - (1 - \frac{1}{2^{2k}})\binom{2k}{2a+2k-2n+1}\right]\mathbb{1}_{a+k\geq n}\end{aligned}$$

Corollary 2.8.6. *Let $f(x_1, x_2, x_3) \in \mathfrak{bg}$ be homogeneous of degree $2n + 4$. Let f_{ooe} be the part of f that is odd in x_1 and x_2. Then $\frac{\partial f_{ooe}}{\partial x_2}(x_1, 0, x_3) \in V_{\bar{p}}$ where*

$$V_{\bar{p}} := \left\langle (x_1^{2k} - x_3^{2k})\bar{p}_{2n-2k+1}(x_1, x_3) - (x_1^{2n-2k} - x_3^{2n-2k})\bar{p}_{2k+1}(x_1, x_3) - \frac{x_1x_3^2}{2}(x_1^{2k}x_3^{2n-2k} - x_1^{2n-2k}x_3^{2k})\right\rangle_{\mathbb{Q}}$$

where $1 \leq k < \frac{n}{2}$ and

$$\bar{p}_{2k+1}(x, y) := \frac{xy^2}{2}\left((x + y)^{2k} + (x - y)^{2k}\right) - \frac{x^2y}{2}\left(1 - \frac{1}{2^{2k}}\right)\left((x + y)^{2k} - (x - y)^{2k}\right).$$

Proof. Noting that, for $f(x_1, x_2, x_3) \in \mathfrak{bg}$, the coefficient of $x_1x_2x_3^{2n+2}$ vanishes as a consequence of the dihedral symmetries in $\mathfrak{rbg}$. Hence, if c_a is the coefficient of $x_1^{2a+3}x_2x_3^{2n-2a}$, we can write

$$\sum_{a=0}^{n-1} c_a x_1^{2a+3} x_3^{2n-2a} = \frac{1}{2}\left(\frac{\partial f}{\partial x_2}(x_1,0,x_3) - \frac{\partial f}{\partial x_2}(-x_1,0,x_3)\right) = \frac{\partial f_{ooe}}{\partial x_2}(x_1,0,x_3).$$

Explicitly summing these polynomials, we see that for $f = \{p_{2n-2k+1}, p_{2k+1}\}$, we must have

$$\frac{\partial f_{ooe}}{\partial x_2}(x_1,0,x_3) = (x_1^{2k}-x_3^{2k})(\bar{p}_{2n-2k+1}(x_1,x_3)-\frac{x_1x_3^{2n-2k+2}}{2})-(x_1^{2n-2k}-x_3^{2n-2k})(\bar{p}_{2k+1}(x_1,x_3)-\frac{x_1x_3^{2k+2}}{2})$$

Simplifying this, we obtain an element of $V_{\bar{p}}$. Hence, general $f(x_1,x_2,x_3) \in \mathfrak{bg}$ of degree $2n+4$ must have $\frac{\partial f}{\partial x_2}(x_1,0,x_3) \in V_{\bar{p}}$. □

An equivalent statement is that $r(x_1,x_2,x_3) \in \mathfrak{rbg}$ must satisfy

$$x_1^2 x_3 r_{oeo}(x_1,0,x_3) - x_1 x_3^2 r_e(x_1,0,x_3) \in V_{\bar{p}}$$

where r_{oeo} is the part of r that is odd in x_1 and x_3, and r_e is the totally even part of r. We claim that this condition determines the totally even part of $r(x_1,x_2,x_3) = \frac{f(x_1,x_2,x_3)}{x_1,x_2,x_3}$.

Proposition 2.8.7. *Let V be the vector space of $r(x_1,x_2,x_3) \in \mathbb{Q}[x_1,x_2,x_3]$ that are homogeneous of degree $2n+2$ and that satisfy*

(1): $r(x_1,x_2,x_3) = r(x_2,x_3,x_1) = -r(x_3,x_2,x_1)$,

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

(3): $\frac{\partial^4 r}{\partial x_1^4} + \frac{\partial^4 r}{\partial x_2^4} + \frac{\partial^4 r}{\partial x_3^4} - 2\frac{\partial^4 r}{\partial x_1^2\partial x_2^2} - 2\frac{\partial^4 r}{\partial x_2^2\partial x_3^2} - 2\frac{\partial^4 r}{\partial x_3^2\partial x_1^2} = 0$,

(4): $x_1^2 x_3 r_{oeo}(x_1,0,x_3) - x_1 x_3^2 r_e(x_1,0,x_3) \in V_{\bar{p}}$,

(5): $x_1^2 x_3 r_{oeo}(x_1,0,x_3) - x_1 x_3^2 r_e(x_1,0,x_3) = 0$ *only if* $r(x_1,x_2,x_3) = 0$.

Let $d_{2,2n}$ be the dimension of the degree $2n$ piece of $\mathfrak{rbg}_2$, i.e. the dimension of the weight $2n+2$ part of $\mathfrak{bg}_2$. Then dim $V = d_{2,2n}$.

Proof. First note that, following Propositions 2.8.1 and 2.8.2, it is sufficient to show that the totally even part r_e of $r \in V$ is determined by $r(x_1,x_2,x_3)-r_e(x_1,x_2,x_3)$. Furthermore, by Lemma 2.8.3, it is sufficient to show that $r_e(x_1,0,x_3)$ is determined by the odd part of

$r(x_1,x_2,x_3)$. By (4), we must have $\beta_k \in \mathbb{Q}$ such that

$$\begin{aligned}
&x_1^2x_3r_{oeo}(x_1,0,x_3) - x_1x_3^2r_e(x_1,0,x_3) = \\
&\sum_{0<k<n/2} \beta_k(x_1^{2k}-x_3^{2k})(x_1^2x_3\rho_{2n-2k+1,o}(x_1,x_3) - x_1x_3^2\rho_{2n-2k+1,e}(x_1,x_3)) \\
&-\beta_k(x_1^{2n-2k}-x_3^{2n-2k})(x_1^2x_3\rho_{2k+1,o}(x_1,x_3) - x_1x_3^2\rho_{2k+1,e}(x_1,x_3)) \\
&-\beta_k x_1x_3^2(x_1^{2k}x_3^{2n-2k} - x_1^{2n-2k}x_3^{2k})
\end{aligned}$$

where

$$\begin{aligned}
\rho_{2m+1,o}(x,y) &:= \left(1-\frac{1}{2^{2m}}\right)\left((x+y)^{2m}-(x-y)^{2m}\right) \\
\rho_{2m+1,e}(x,y) &:= \left((x+y)^{2m}+(x-y)^{2m}\right).
\end{aligned}$$

Dividing through by x_1x_3, we obtain

$$\begin{aligned}
&x_1r_{oeo}(x_1,0,x_3) - x_3r_e(x_1,0,x_3) = \\
&\sum_{0<k<n/2} \beta_k(x_1^{2k}-x_3^{2k})(x_1\rho_{2n-2k+1,o}(x_1,x_3) - x_3\rho_{2n-2k+1,e}(x_1,x_3)) \\
&-\beta_k(x_1^{2n-2k}-x_3^{2n-2k})(x_1\rho_{2k+1,o}(x_1,x_3) - x_3\rho_{2k+1,e}(x_1,x_3)) \\
&-\beta_k x_3(x_1^{2k}x_3^{2n-2k} - x_1^{2n-2k}x_3^{2k}).
\end{aligned}$$

Swapping x_1 and x_3, and adding this to the original equation, we then obtain

$$\begin{aligned}
&(x_1-x_3)r_{oeo}(x_1,0,x_3) + (x_1-x_3)r_e(x_1,0,x_3) = \\
(x_1-x_3)&\sum_{0<k<n/2} \beta_k(x_1^{2k}-x_3^{2k})(\rho_{2n-2k+1,o}(x_1,x_3) + \rho_{2n-2k+1,e}(x_1,x_3)) \\
&-\beta_k(x_1^{2n-2k}-x_3^{2n-2k})(\rho_{2k+1,o}(x_1,x_3) + \rho_{2k+1,e}(x_1,x_3)) \\
&+\beta_k(x_1^{2k}x_3^{2n-2k} - x_1^{2n-2k}x_3^{2k}).
\end{aligned}$$

Dividing through by $(x_1 - x_3)$ and equating even and odd parts, we find

$$\begin{aligned}
r_{oeo}(x_1, 0, x_3) = \sum_{0<k<n/2} & \beta_k(x_1^{2k} - x_3^{2k})\rho_{2n-2k+1,o}(x_1, x_3) \\
& - \beta_k(x_1^{2n-2k} - x_3^{2n-2k})\rho_{2k+1,o}(x_1, x_3), \\
r_e(x_1, 0, x_3) = \sum_{0<k<n/2} & \beta_k(x_1^{2k} - x_3^{2k})\rho_{2n-2k+1,e}(x_1, x_3) \\
& - \beta_k(x_1^{2n-2k} - x_3^{2n-2k})\rho_{2k+1,e}(x_1, x_3) + \beta_k(x_1^{2k}x_3^{2n-2k} - x_1^{2n-2k}x_3^{2k}).
\end{aligned}$$

Comparing coefficients for the odd part, we obtain equations for β_k. We claim these equations determine β_k completely.

Suppose otherwise. Then there exist non-trivial $\{\beta_k\} \subset \mathbb{Q}$ such that

$$\sum_{0<k<n/2} \beta_k(x_1^{2k} - x_3^{2k})\rho_{2n-2k+1,o}(x_1, x_3) - \beta_k(x_1^{2n-2k} - x_3^{2n-2k})\rho_{2k+1,o}(x_1, x_3) = 0.$$

Let $r_{2s+1}(x_1, x_2) = \frac{p_{2s+1}(x_1,x_2)}{x_1x_2(x_1-x_2)}$, and consider

$$r(x_1, x_2, x_3) = \sum_{0<k<n/2} \beta_k\{r_{2n-2k+1}, r_{2k+1}\}(x_1, x_2, x_3).$$

By the above calculation, and our assumption, we must have

$$r_{oeo}(x_1, 0, x_3) = 0.$$

However, from the proof of Proposition 2.8.1, $r_{oeo}(x_1, x_2, x_3)$ can uniquely determined from $r_{oeo}(x_1, 0, x_3)$, and so we must have $r_{oeo}(x_1, x_2, x_3) = 0$, and so $r(x_1, x_2, x_3) = r_e(x_1, x_2, x_3)$. Proposition 2.8.1 also tells us that the projection map

$$\begin{aligned}
\pi_o : \mathfrak{rbg}_{2,2n} &\to V_o \\
r(x_1, x_2, x_3) &\mapsto r(x_1, x_2, x_3) - r_e(x_1, x_2, x_3)
\end{aligned}$$

is an isomorphism. Thus, if $r(x_1, x_2, x_3) = r_e(x_1, x_2, x_3)$, we must have $r(x_1, x_2, x_3) = 0$, giving a relation in a free Lie algebra. Hence, no such $\{\beta_k\}$ exist. Therefore, given $r_{oeo}(x_1, x_2, x_3)$, the corresponding β_k are uniquely determined, uniquely determining $r_e(x_1, x_2, x_3)$.

The result follows. □

Remark 2.8.8. While we did not explicitly use (3) in the above proof, it is essential in constructing the isomorphisms. Indeed, if we removed (3) as a constraint, numerical calculations suggest that comparing coefficients leaves us with a single degree of freedom in our choice of β_k. The author believes to to be related to the fact that the vector space $V_{\overline{p}}$ only contains information about convergent MZVs.

2.9 Double shuffle and associator relations in the block graded algebra

In general, it is quite difficult to produce graded analogues of previously known relations. We can, similarly to Corollary 2.5.2, 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 $\mathrm{gr}_{\mathcal{B}}(\Delta_1)$ with projection onto the second component.

Lemma 2.9.1. *For* $f(x_1, \ldots, x_n) \in \mathfrak{bg}$

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

However, the shuffle equations do not, in general, behave well with respect to the block filtration. Attempting similar with the stuffle equations, we find that is is difficult to encode stuffle relations as functional equations satisfied by elements of $\mathfrak{bg}$. However, returning to direct computations with multiple zeta values, we find that the stuffle equations behave very nicely with respect to the block filtration. We first note that, for convergent MZVs, computation of block degree is a function of the arguments.

Lemma 2.9.2. *The block degree of* $\zeta^{\mathfrak{m}}(n_1, \ldots, n_k)$ *is given by* $\sum_{i=1}^{k} |n_i - 2|$.

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

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

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 2.9.3. 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 $\deg_{\mathcal{B}}(\zeta^{\mathfrak{m}}(n_1, \dots, n_k) = n_1 + \cdots + n_k - 2k$, i.e block degree is weight minus twice depth. This is a special case of a more general relation

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

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 2.9.4. *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 $m_{k+1} = \ldots = m_l = 0$. Then*

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

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 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 2.9.5. We can, in fact, extend Proposition 2.9.4 to allow m_i, n_j to be equal to 1, in light of Remark 2.9.3, 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 2.9.6. *For any interval* $I = \{k, k+1, \ldots, k+l\} \subset \{1, \ldots, n\}$ *of cardinality at least 2, and any* $f(x_1, \ldots, x_n) \in \mathfrak{bg}$*, we have*

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

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

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

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

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

at $(z_1, \ldots, z_n)$ 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.

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

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

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

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

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

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. □

Proposition 2.9.8. *The set of equations obtained by extracting the coefficients of each monomial in the linearised hexagon equation*

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

contains 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 $\mathrm{I}^{\mathfrak{m}}(0; w; 1)$. From $\phi(e_1, -e_0 - e_1)$, we obtain a sum of terms of the form $\mathrm{I}^{\mathfrak{m}}(0; u; 1)$ where u is a word with e_0 only where w has e_1. From $\phi(-e_0 - e_1, e_0)$, we obtain a sum of terms of the form $\mathrm{I}^{\mathfrak{m}}(0; v; 1)$ where v is a word with 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

$$e_0^k e_1^{n-k},$$
$$e_0^i e_1^j e_0^{n-i-j},$$
$$e_1^i e_0^j e_1^{n-i-j},$$

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 2.9.7, 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. □

Remark 2.9.9. Writing down block graded versions of the pentagon equation would be an interesting challenge. Our naive approach to the hexagon equations provides little information, but numerical evidence suggests that naively block grading the pentagon equations could produce a new set of relations.

2.10 Deriving the Ihara action formula

For elements of the double shuffle Lie algebra, the (linearised) Ihara action is given by the following [13]:

Proposition 2.10.1. *For $\sigma \in Lie[e_0, e_1]$, $u \in \{e_0, e_1\}^\times$, the linearised Ihara action is given recursively by*

$$\sigma \circ e_0^n e_1 u := e_0^n \sigma e_1 u - e_0^n e_1 \sigma^* u + e_0^n e_1 (\sigma \circ u) \tag{2.10.1}$$

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

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

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 (2.10.1) shows $\epsilon_i = 0$, as σ does not 'insert' between adjacent e_0. If $u_i = u_{i+1} = e_1$, then our recursion gives us terms of the form

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

As, for $\sigma \in \mathrm{Lie}[e_0, e_1]$, $\sigma + \sigma^* = 0$, 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 σ 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

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

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

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

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, i.e. $e_0 u e_1 = b_1 \dots b_n$, represented by 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 $\sigma \in \mathrm{Lie}[e_0, e_1]$ 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 σ inserts into $b_{n-1}b_n$. Indeed, they will agree under this swapping until we consider terms in which σ inserts beyond the end of b_{n-1}. Thus, it suffices to show that the formula holds for a word $e_0ue_1 = b_1b_2$ of block degree 1.

We have 2 cases: the repeated letter in e_0ue_1 is e_0, or it is e_1. In the first case, $u = (e_1e_0)^k e_0(e_1e_0)^l$ and

$$\begin{aligned}\sigma \circ u = &\sum_{i=0}^{k}(e_1e_0)^i\sigma(e_1e_0)^{k-i}e_0(e_1e_0)^l + \sum_{i=0}^{k-1}(e_1e_0)^i e_1\sigma^* e_0(e_1e_0)^{k-1-i}e_0(e_1e_0)^l \\ &+ \sum_{i=0}^{l}(e_1e_0)^k e_0(e_1e_0)^i\sigma(e_1e_0)^{l-i} + \sum_{i=0}^{l-1}(e_1e_0)^k e_0(e_1e_0)^i e_1\sigma^* e_0(e_1e_0)^{l-1-i}\end{aligned}$$

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

$$\begin{aligned}(f \circ g)(x_1, \ldots, x_{m+1}) = &\frac{f(x_1, \ldots, x_m)}{x_1^2 - x_m^2}\left((\frac{x_1}{x_m})^{2k} - 1 + (-1)^{m+1}(\frac{x_1}{x_m})^{2k+1} - (-1)^{m+1}\frac{x_1}{x_m}\right) g(x_m, x_{m+1}) \\ &+ \frac{f(x_2, \ldots, x_{m+1})}{x_2^2 - x_{m+1}^2}\left((\frac{x_2}{x_{m+1}})^{2l+2} - 1 + (-1)^{m+1}(\frac{x_2}{x_{m+1}})^{2l+1} - (-1)^{m+1}\frac{x_2}{x_{m+1}}\right) g(x_1, x_{m+1}).\end{aligned}$$

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

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

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

$$\begin{aligned}(f \circ g)(x_1, \ldots, x_{m+1}) = (-1)^{(0)(m+1)}\frac{f(x_1, \ldots, x_m)}{x_1^2 - x_m^2}&\Bigg(g(\bar{x}_1, x_{m+1}) + (-1)^{m+1}\frac{x_m}{x_1}g(\bar{x}_1, x_{m+1})\\ &-g(x_m, x_{m+1}) + (-1)^{m+1}\frac{x_m}{x_{m+1}}g(x_m, x_{m+1})\Bigg)\\ &+ (-1)^{m+1}\frac{f(x_2, \ldots, x_{m+1})}{x_2^2 - x_{m+1}^2}\Bigg(g(\bar{x}_1, \bar{x}_2) - (-1)^{m+1}\frac{x_{m+1}}{x_2}g(\bar{x}_1, \bar{x}_2)\\ &-g(\bar{x}_1, x_{m+1}) + (-1)^{m+1}\frac{x_2}{x_{m+1}}g(\bar{x}_1, x_{m+1})\Bigg)\end{aligned}$$

giving the desired formula. The second case follows similarly.

Hence, our general formula is $(f \circ g)(x_1, \ldots, x_{m+n-1}) = A \pm B \pm C$, where

$$\begin{aligned}A = \sum_{i=1}^{n-2}&(-1)^{(m+1)(i-1)}\frac{f(x_i, x_{i+1}, \ldots, x_{i+m-1})}{x_i^2 - x_{i+m-1}^2}\\ \times&\Bigg((1 + (-1)^{m+1}\frac{x_{i+m-1}}{x_i})g(\bar{x}_1, \ldots, \bar{x}_i, x_{i+m}, \ldots, x_{m+n-1})\\ -&(1 + (-1)^{m+1}\frac{x_i}{x_{i+m-1}})g(\bar{x}_1, \ldots, \bar{x}_{i-1}, x_{i+m-1}, \ldots, x_{m+n-1})\Bigg),\end{aligned}$$

$$\begin{aligned}B = &(-1)^{(m+1)(n-2)}\frac{f(x_{n-1}, \ldots, x_{m+n-2})}{x_{n-1}^2 - x_{n+m-2}^2}\\ \times&\Bigg((1 + (-1)^{m+1}\frac{x_{n+m-2}}{x_{n-1}})g(\bar{x}_1, \ldots, \bar{x}_{n-1}, x_{m+n-1})\\ -&(1 + (-1)^{m+1}\frac{x_{n-1}}{x_{n+m-2}})g(\bar{x}_1, \ldots, \bar{x}_{n-2}, x_{n+m-2}, x_{m+n-1})\Bigg),\end{aligned}$$

$$\begin{aligned}C = &(-1)^{(m+1)(n-1)}\frac{f(x_n, \ldots, x_{m+n-1})}{x_n^2 - x_{m+n-1}^{"}}\\ \times&\Bigg((1 + (-1)^{m+1}\frac{x_{n+m-1}}{x_n})g(\bar{x}_1, \ldots, \bar{x}_n)\\ -&(1 + (-1)^{m+1}\frac{x_n}{x_{n+m-1}})g(\bar{x}_1, \ldots, \bar{x}_{n-1}, x_{m+n-1})\Bigg),\end{aligned}$$

and the signs of B and C agree. To fix this sign, we need only to consider the sign of the term corresponding to $(\frac{x_{n-1}}{x_{m+n-2}})^2\frac{f(x_{n-1},\ldots,x_{m+n-2})g(x_1,\ldots,x_{n-2},x_{m+n-2},x_{m+n-1})}{x_{m+n-2}^2}$. This corresponds to inserting σ after the first two letters of the $(n-1)^{th}$ block. The sign will be positive if this block starts with an e_1 and must have the same sign as $(-1)^{m+1}$ otherwise. Let $g(x_1, \ldots, x_n) = x_1^{d_1} \ldots x_n^{d_n}$. Then by Lemma 2.1.10 the $(n-1)^{th}$ block starts with e_0 if $d_1 + \ldots + d_{n-2} \equiv n - 2 \pmod 2$, and e_1 otherwise. Thus, the sign of the term corresponding to $(\frac{x_{n-1}}{x_{m+n-2}})^2\frac{f(x_{n-1},\ldots,x_{m+n-2})g(x_1,\ldots,x_{n-2},x_{m+n-2},x_{m+n-1})}{x^2_{m+n-2}}$ is $(-1)^{(m-1)(1+d_1+\ldots+d_{n-2}-n+2)}$. 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 (2.3.2), 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 2.10.3. *The automorphism $\mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle e_0, e_1\rangle$ given by $e_1 \mapsto -e_1$, is equivalent under the isomorphism (2.3.1) to the map*

$$\begin{aligned} &\mathbb{Q}[x_1,\ldots,x_n] \to \mathbb{Q}[x_1,\ldots,x_n] \\ &f(x_1,\ldots,x_n) \mapsto (-1)^{\lceil \frac{l}{2}\rceil} f(-x_1,x_2,\ldots,(-1)^n x_n) \end{aligned} \tag{2.10.2}$$

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 $\pi_{\mathrm{bl}}(w) = x_1^{d_1}\ldots x_n^{d_n}$, this congruence holds

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

We will induct on the number of blocks in e_0we_1. If e_0we_1 consists of a single block, then $e_0we_1 = (e_0e_1)^{\frac{l}{2}+1}$, and so $d = \frac{l}{2}$, and $d_1 = l+2$. Thus the result holds.

Suppose the result holds for w such that e_0we_1 consists of n blocks. Let $e_0we_1 = w'w_{d_{n+1}}$ 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 $\pi_{\mathrm{bl}}(w) = x_1^{d_1}\ldots x_n^{d_n}x_{n+1}^{d_{n+1}}$.

If l' is even, then $w' = e_0ue_1$ consists of $n \equiv 1 \pmod 2$ blocks, and d_{n+1} must be odd. So, by induction,

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

Thus

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

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

Applying this transformation, and simplifying, we obtain Proposition 2.3.6, giving the formula

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

2.11 The Ihara action in noncommuting variables

Using the isomorphism (2.4.1), we can define a vector space isomorphism

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

and hence an injection

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

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

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

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

Lemma 2.11.1. *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 $f\in Q[x_1,\ldots,x_m]$, $F\in\mathbb{Q}[x_1,\ldots,x_n]$, we define

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

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

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

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

$$f\circ x_1^n = \frac{f(x_1,\ldots,x_m)}{x_1-x_m}\left(x_1^{n-1}-x_m^{n-1}\right) = f(x_1,\ldots,x_m)\sum_{i+j=n-2}x_1^i x_m^j$$

Thus, we have that

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

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

This also provides us with an alternative proof of Theorem 2.4.3, via the following equivalent statement.

Proposition 2.11.2. *The image of every $\sigma \in \mathfrak{bg}$ 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, σ primitive is equivalent to $\sigma \in \mathrm{Lie}[Z]$. 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 $\sigma,\ \psi \in \mathrm{Lie}[Z]$, that $\sigma \circ \psi \in \mathrm{Lie}[Z]$. In particular, as we are interested in the image of $\mathfrak{bg}$, we may take σ to be in this image, and in fact, by associativity of the Ihara action, we may take σ to be of block degree 1. Finally, since the Ihara action is linear and a derivation, it suffices to show

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

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 σ in the image of $\mathfrak{bg}$, and $\psi \in \mathrm{Lie}[Z]$, $\sigma \circ \psi \in \mathrm{Lie}[Z]$, and we can therefore conclude that the image of $\mathfrak{bg}$ is contained in $\mathrm{Lie}[Z]$. □

Remark 2.11.3. Careful comparison of this proof, and that of Theorem 2.4.3 reveal that these give two slightly distinct proofs, but they fundamentally rely on the same properties. The proof of Proposition 2.11.2 requires that the Ihara action be a derivation for concatenation, while the proof of Theorem 2.4.3 requires that in each

$$\frac{f(x_i, x_{i+1})}{x_i - x_{i+1}} \times \hat{g}(x_1, \ldots, x_n)$$

appearing in the formula for the Ihara action, the $\hat{g}$ differs from g by the degree of at most 1 variable. This is equivalent to being a derivation, and, as such, these proofs utilise no different properties. The key distinction is that the proof of Proposition 2.11.2 shows that each summand in $f \circ g$ satisfies the block shuffle property, while the proof of Theorem 2.4.3 only shows that the total sum satisfies the block shuffle property.

Chapter 3

Block graded relations and known relations

3.1 The double shuffle relations in the block graded algebra

As alluded previously, block graded double shuffle relations, in particular the shuffle relations, cannot easily be written down. However, in low block degrees we can show that the block graded analogues of relations of the form

$$\zeta^{\mathfrak{m}}(u ⧢ v) = 0 \text{ or } \zeta^{\mathfrak{m}}(u \star v) = 0 \text{ modulo products}$$

follow from the relations discussed in Remark 2.7.4. These do not encompass all block graded double shuffle relations. For example, in block degree 2, we find the mod products relation

$$2\zeta(3,3,2) + \zeta(3,2,3) = -\frac{7}{2}\left(2\zeta(4,2,2) + \zeta(2,4,2)\right)$$

as a consequence of the double shuffle relations, but this is not implied by the relations discussed in Remark 2.7.4. Nevertheless, it is an interesting exercise.

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

$$\sum_{\substack{0\leq i\leq k-1\\ n_{i+1}\neq 1}} \zeta^{\mathfrak{bl}}(n_1,\dots,n_i,1,n_{i+1},\dots,n_k) - \sum_{\substack{1\leq i\leq k\\ n_i\neq 1}} \zeta^{\mathfrak{bl}}(n_1,\dots,n_i+1,\dots,n_k) = 0 \tag{3.1.1}$$

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

Lemma 3.1.1. *The Hoffman regularisation relation holds for block graded multiple zeta values.*

Proof. Consider $-\mathrm{I}^{\mathfrak{bl}}(z_1 ш z_{i_1} \dots z_{i_n}) = 0$, 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

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

Let $w_1, w_2 \in \mathbb{Q}\langle e_0, e_1\rangle$ be the monomials defined by the correspondences $e_0 w_1 \leftrightarrow z_1 z_{i_1} \dots z_{i_n}$ and $w_2 e_1 \leftrightarrow z_{i_1} \dots z_{i_n} z_1$. Using shuffle regularisation

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

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

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

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

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

corresponds bijectively to

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

and the set

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

corresponds bijectively to

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

and thus, $\mathrm{I}^{\mathfrak{bl}}(z_1 ⧢ z_{i_1}\dots z_{i_n})=0$ is equivalent to equation (3.1.1). □

We now turn to the double shuffle relations in block degree 1. The shuffle relations tell us that $\mathrm{I}^{\mathfrak{l}}(0;u ⧢ v;1)=0$ 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 and v contains an e_0e_1 or an e_1e_0 as a subword.

Thus in $e_0(u ⧢ v)e_1$, we can find a word containing both an e_1^2 and an e_0^2 that were not in v, and so $\deg_{\mathcal{B}}(u ⧢ v)\geq\deg_{\mathcal{B}}(v)+2$, 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 arise from $\zeta^{\mathfrak{m}}(u\star v)$ where $\deg_{\mathcal{B}}(u)=0$, $\deg_{\mathcal{B}}(v)=1$, and so $u=y_2^n$, and $v=y_2^ay_ky_2^b$ 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 naive 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 $\mathrm{I}^{\mathfrak{a}}(e_1e_0 ⧢ (e_1e_0)^n)=0$, and $\zeta^{\mathfrak{m}}(y_2\star y_2^n)=0$ modulo products. We first consider the stuffle relation.

Taking the block graded piece, we obtain that

$$\sum_{i=1}^{n}\zeta^{\mathfrak{m}}(\{2\}^{i-1},4,\{2\}^{n-i})=0\text{ modulo products}$$

which is equivalent to

$$\sum_{i=1}^{n}\mathrm{I}^{\mathfrak{bl}}(z_{2i+1}z_1z_{2n-2i+2})=0,$$

which would follow from the statement that, for all $f(x_1,x_2,x_3)\in\mathfrak{bg}$, $\frac{\partial f}{\partial x_2}(x_1,0,x_1)=0$.

We know that $f(x_1, x_2, x_3) = x_1x_2x_3(x_1 - x_3)r(x_1, x_2, x_3)$, and hence

$$\frac{\partial f}{\partial x_2}(x_1, 0, x_3) = x_1x_3(x_1 - x_3)r(x_1, 0, x_3)$$

from which the claim obviously follows.

Now, considering $\mathrm{I}^{\mathfrak{a}}(e_1e_0 ⧢ (e_1e_0)^n)$, and taking the block degree 2 piece, we obtain that

$$\sum_{i=0}^{n-1}\sum_{j=0}^{n-i-1} \mathrm{I}^{\mathfrak{bl}}((e_1e_0)^i e_1^2 (e_0e_1)^j e_0^2 (e_1e_0)^{n-i-j-1}) = 0,$$

or equivalently

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

which we can rewrite once more as

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

which follows from the statement that, for all $f(x_1, x_2, x_3) \in \mathfrak{bg}$, $f_{eee}(x, x, x) = 0$, 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 $f(x_1, x_2, x_3) = x_1x_2x_3(x_1 - x_3)r(x_1, x_2, x_3)$, for $r \in \mathfrak{rbg}$, we have that

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

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

3.2 The Ohno-Zagier relations in the block graded algebra

Recall in Remark 2.9.3, we noted that

$$Weight - Block = 2(Depth - Ones)$$

This quantity on the right, *Depth−Ones*, is precisely the number of $n_i > 1$ in $\zeta^{\mathfrak{m}}(n_1, \ldots, n_k)$ and is known as the *height*. Thus a relation among motivic multiple zeta values is homogeneous in block degree if and only if it is homogeneous in height. A large family of such relations come from the Ohno-Zagier relations [36].

Theorem 3.2.1. *Let $I(n,k,h)$ be the set of multi-indices $(n_1, \ldots, n_k) \in \mathbb{N}^k$ with exactly h of the n_i greater than 1, $n_k > 1$ and $n_1 + \cdots + n_k = n$. Then*

$$\sum_{(n_1,\ldots,n_k)\in I(n,k,h)} \zeta(n_1, \ldots, n_k) = 0 \textit{ modulo products.}$$

We can show that this is a consequence of the homogeneity of elements of $\mathfrak{bg}$, and Lemma 2.1.10, modulo terms of lower block degree.

Proposition 3.2.2.

$$\sum_{(n_1,\ldots,n_k)\in I(n,k,h)} \zeta^{\mathfrak{m}}(n_1, \ldots, n_k) = 0 \textit{ modulo products and terms of lower block degree}$$

Proof. First note that the block degree of such elements is $n - 2h$, and that the depth of $\mathrm{I}^{\mathfrak{m}}(x_{b_1} \ldots x_{b_m})$ is equal to

$$\lfloor \frac{n}{2} \rfloor + \sum_{i=1}^{m-1} \mathbb{1}_{b_1+\cdots+b_i \equiv i+1 \pmod 2} - \sum_{i=1}^{m-1} \mathbb{1}_{b_1+\cdots+b_i \equiv i \pmod 2}.$$

To see this, note that every word w in $\{e_0, e_1\}$ can be written uniquely as a word in $\{e_0e_1, e_1e_0, e_1^2, e_0^2\}$ with a possible e_0 or e_1 appended to the end. $\lfloor \frac{n}{2} \rfloor$ counts the number of pairs. $\sum_{i=1}^{m-1} \mathbb{1}_{b_1+\cdots+b_i \equiv i+1 \pmod 2}$ counts the number of e_1^2 (and whether the word ends on e_1), and $\sum_{i=1}^{m-1} \mathbb{1}_{b_1+\cdots+b_i \equiv i \pmod 2}$ counts the number of e_0^2. Thus, the depth of an element with block decomposition $x_{b_1} \ldots x_{b_m}$ is uniquely determined by the parity sequence $(p_1, \dots, p_m) \equiv (b_1, \dots, b_m) \pmod 2$. Thus, we have that

$$\sum_{(n_1,\dots,n_k)\in I(n,k,\frac{n-b}{2})} \zeta^{\mathfrak{m}}(n_1,\dots,n_k) = \pm \sum_{\substack{(p_1,\dots,p_m)\\ \text{corresponding to}\\ \text{depth } d}} \sum_{\substack{b_1+\cdots b_m=n+2\\ (b_1,\dots,b_m)\equiv(p_1,\dots,p_m)\\ b_1,b_m>1}} \mathrm{I}^{\mathfrak{bl}}(x_{b_1}\dots x_{b_m})$$

Thus, it will be sufficient to show the following, for any parity sequence $(p_1, \dots, p_m) \in \{0,1\}^m$ and and $f(x_1, \dots, x_m) \in \mathfrak{bg}$.

$$\begin{aligned} f_{(p_1,\dots,p_m)}(x, x, \dots, x) &= 0, \\ \frac{\partial f_{(p_1,\dots,p_m)}}{\partial x_1}(0, x, \dots, x) &= 0 \text{ if } p_1 = 0, \\ \frac{\partial f_{(p_1,\dots,p_m)}}{\partial x_m}(x, \dots, x, 0) &= 0 \text{ if } p_m = 0, \\ \frac{\partial^2 f_{(p_1,\dots,p_m)}}{\partial x_1 \partial x_m}(0, x, \dots, x, 0) &= 0 \text{ if } p_1 = p_m = 0. \end{aligned}$$

Here $f_{(p_1,\dots,p_m)}(x_1, \dots, x_n)$ is the part of f such that the map $x_i \mapsto -x_i$ sends $f_{(p_1,\dots,p_m)} \mapsto (-1)^{p_i} f_{(p_1,\dots,p_m)}$.

$$f_{(p_1,\dots,p_m)}(x_1, \dots, x_m) = \frac{1}{2^m} \sum_{(i_1,\dots,i_m)\in\{0,1\}^m} (-1)^{\sum p_j i_j} f((-1)^{i_1} x_1, \dots, (-1)^{i_m} x_m).$$

Recall that we must have, by Lemma 2.1.10, we must have $n \equiv m + 1 \pmod 2$. Thus, using the homogeneity of f, we can write

$$\begin{aligned} f_{(p_1,\dots,p_m)}(x, \dots, x) &= \frac{1}{2^m} \sum_{(i_1,\dots,i_m)\in\{0,1\}^m} (-1)^{\sum p_j i_j} f((-1)^{i_1} x, \dots, (-1)^{i_m} x) \\ &= \frac{1}{2^{n+1}} \sum_{(i_1,\dots,i_m)\in\{0,1\}^m} (-1)^{\sum p_j i_j} f((-1)^{i_1} x, \dots, (-1)^{i_m} x) \\ &\qquad + (-1)^{\sum p_j (1-i_j)} f((-1)^{1-i_1} x, \dots, (-1)^{1-i_m} x) \\ &= \frac{1}{2^{n+1}} \sum_{(i_1,\dots,i_m)\in\{0,1\}^m} (-1)^{\sum p_j i_j} f((-1)^{i_1} x, \dots, (-1)^{i_m} x) \\ &\qquad + (-1)^{n+m+\sum p_j i_j} f((-1)^{i_1} x, \dots, (-1)^{i_m} x) \\ &= \frac{1}{2^{n+1}} \sum_{(i_1,\dots,i_m)\in\{0,1\}^m} (-1)^{\sum p_j i_j} f((-1)^{i_1} x, \dots, (-1)^{i_m} x) \\ &\qquad + (-1)^{1+\sum p_j i_j} f((-1)^{i_1} x, \dots, (-1)^{i_m} x) \end{aligned}$$

$$= 0.$$

We similarly see that

$$\begin{aligned}\frac{\partial f_{(p_1,\ldots,p_m)}}{\partial x_1}(0,x,\ldots,x) &= \frac{1}{2^m}\sum_{(i_1,\ldots,i_m)\in\{0,1\}^m}(-1)^{(p_1+1)i_1+\sum_{i>1}p_j i_j}\frac{\partial f}{\partial x_1}(0,(-1)^{i_2}x,\ldots,(-1)^{i_m}x)\\ &= \frac{1}{2^m}\sum_{(i_1,\ldots,i_m)\in\{0,1\}^m}(-1)^{\sum_{i>1}p_j i_j}\frac{\partial f}{\partial x_1}(0,(-1)^{i_2}x,\ldots,(-1)^{i_m}x)\\ &= 0\end{aligned}$$

as, if $p_1 = 1$, $\frac{\partial f_{(p_1,\ldots,p_m)}}{\partial x_1}(0,x_2,\ldots,x_m)$ is homogeneous of degree congruent to m mod 2.

Near identical arguments show the final two equalities. Therefore we can conclude

$$\sum_{(n_1,\ldots,n_k)\in I(n,k,h)}\zeta^{\mathfrak{m}}(n_1,\ldots,n_k) = 0 \text{ modulo products and terms of lower block degree.}$$

$\square$

Chapter 4

An ungraded block shuffle

We wish to extend relations among block graded multiple zeta values to motivic multiple zeta values, modulo products. For example, the work of Charlton [14] suggests that cyclic insertion holds at the level of motivic multiple zeta values. We shall first introduce an extension of the block shuffle relation to motivic multiple zeta values, defined in work due to Hirose and Sato [29].

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

$$\begin{aligned}
&z_m u \mathbin{\hat{\sqcup\!\sqcup}} z_n v := z_m(u \mathbin{\hat{\sqcup\!\sqcup}} z_n v) + z_n(z_m u \mathbin{\hat{\sqcup\!\sqcup}} v) - L_{m+n}(u \mathbin{\hat{\sqcup\!\sqcup}} v),\\
&u \mathbin{\hat{\sqcup\!\sqcup}} 1 := 1 \mathbin{\hat{\sqcup\!\sqcup}} u := u,
\end{aligned}$$

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 4.0.3. *Let $u, v \in \mathbb{Q}\langle Z\rangle$ be such that (u, v) is not equal to $(z_1^m, z_1^a z_2 z_1^b)$ or $(z_1^a z_2 z_1^b, z_1^m)$ for any $m > 0,\ a, b \geq 0$. Then*

$$I^{\mathfrak{m}}(u \mathbin{\hat{\sqcup\!\sqcup}} v) = 0$$

considered modulo products.

We can translate this into a statement about primitivity of elements of $\mathfrak{g}^{\mathfrak{m}}$ with respect to the following coproduct, which we can readily check to be dual to the above quasi-shuffle product.

Definition 4.0.4. Define a coproduct on $\mathbb{Q}\langle Z\rangle$ by

$$\begin{aligned}
&\Delta_{\mathfrak{bl}}(1) := 1 \otimes 1,\\
&\Delta_{\mathfrak{bl}}(z_n) := \sum_{k\geq 0}(-1)^k \sum_{\substack{i_1+\cdots+i_{2k+1}=n\\ i_j>0}} z_{i_1}\dots z_{i_k}\otimes z_{i_{k+1}}\dots z_{i_{2k+1}} + z_{i_{k+1}}\dots z_{i_{2k+1}}\otimes z_{i_1}\dots z_{i_k}.
\end{aligned}$$

Coassociativity of this coproduct can be checked easily, but tediously, and so we conclude the following.

Lemma 4.0.5. *This quasi-shuffle product is associative.*

We can equivalently reformulate Proposition 4.0.3 as the following statement.

Proposition 4.0.6. *For $n > 0$, define the vector space $V_n := \mathbb{Q}z_1^n \oplus \bigoplus_{a+b=n-2}\mathbb{Q}z_1^a z_2 z_1^b$. Let $\sigma \in \mathfrak{g}^{\mathfrak{m}} \subset \mathbb{Q}\langle Z\rangle$ be an element of weight $N-2$. Then*

$$\Delta_{\mathfrak{bl}}(\sigma) - \sigma\otimes 1 - 1\otimes\sigma \in \sum_{i+j=N} V_i\otimes V_j.$$

While discussing Hirose and Sato's argument is beyond the scope of this thesis, we can prove the following special case of Proposition 4.0.3.

Proposition 4.0.7. *For all $i_1,\dots i_n$ with $i_1, i_n > 1$. $I^{\mathfrak{m}}(z_1 ш z_{i_1}\dots z_{i_n}) = 0$.*

Proof. We claim this is a consequence of Hoffman's regularisation relation. In showing this, we will introduce the following abuse of notation.

$$\begin{aligned}
\mathrm{I}^{\mathfrak{m}}(e_{i_1}e_{i_2}\dots e_{i_n}) &:= \mathrm{I}^{\mathfrak{m}}(0; i_1, i_2, \dots, i_n; 1),\\
\mathrm{I}^{\mathfrak{m}}(n_1,\dots,n_k) &:= (-1)^k\zeta^{\mathfrak{m}}(n_1,\dots,n_k).
\end{aligned}$$

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

$$\mathrm{I}^{\mathfrak{m}}(e_1 \shuffle w) - \mathrm{I}^{\mathfrak{m}}(we_1) = \sum_{i=0}^{k-1} \mathrm{I}^{\mathfrak{m}}(n_1, \ldots, n_i, 1, n_{i+1}, \ldots, n_k) - \sum_{i=1}^{k} \mathrm{I}^{\mathfrak{m}}(n_1, \ldots, n_i + 1, \ldots, n_k).$$

Via the duality relation, the left hand side is equal to

$$(-1)^{N+1} \left(\mathrm{I}^{\mathfrak{m}}(e_0 \shuffle \mathrm{D}w) - \mathrm{I}^{\mathfrak{m}}(e_0 \mathrm{D}w)\right) = (-1)^N \mathrm{I}^{\mathfrak{m}}(z_1 z_{i_n} \ldots z_{i_1}).$$

The sum $\sum_{i=0}^{k-1} \mathrm{I}^{\mathfrak{m}}(n_1, \ldots, n_i, 1, n_{i+1}, \ldots, n_k)$ is equal to

$$\frac{1}{2} \left(\mathrm{I}^{\mathfrak{m}}(e_1 \shuffle w) - \mathrm{I}^{\mathfrak{m}}(we_1) + I_{e_1^2} - I_{e_0^2}\right) = \frac{1}{2} \left((-1)^N \mathrm{I}^{\mathfrak{m}}(z_1 z_{i_n} \ldots z_{i_1}) + I_{e_1^2} - I_{e_0^2}\right)$$

where $I_{e_i^2} := \sum_{\substack{1 \leq k \leq N-1 \\ j_k = j_{k+1} = i}} \mathrm{I}^{\mathfrak{m}}(e_1 \ldots e_{j_k} e_1 e_{j_{k+1}} \ldots e_0)$. By considering when $e_{j_k} = e_{j_{k+1}} = e_1$ can occur, we see that

$$I_{e_1^2} = \sum_{\substack{1 < k \leq n \\ i_1 + \cdots i_k \equiv k+1 \pmod 2}} \mathrm{I}^{\mathfrak{m}}(z_{i_1} \ldots z_{i_k} z_1 \ldots z_{i_n}),$$

and similarly

$$I_{e_0^2} = \sum_{\substack{1 < k \leq n \\ i_1 + \cdots i_k \equiv k \pmod 2}} \mathrm{I}^{\mathfrak{m}}(z_{i_1} \ldots z_{i_{k-1}} z_{i_k + i_{k+1} + 1} z_{i_{k+2}} \ldots z_{i_n}).$$

Hence this first sum is equal to

$$\begin{aligned} &\frac{(-1)^N}{2} \Bigg(\mathrm{I}^{\mathfrak{m}}(z_1 z_{i_n} \ldots z_{i_1}) \\ &+ \sum_{\substack{1 < k \leq n \\ i_1 + \cdots i_k \equiv k+1 \pmod 2}} \mathrm{I}^{\mathfrak{m}}(z_{i_n} \ldots z_{i_{k+1}} z_1 z_k \ldots z_{i_1}) \\ &- \sum_{\substack{1 < k \leq n \\ i_1 + \cdots i_k \equiv k \pmod 2}} \mathrm{I}^{\mathfrak{m}}(z_{i_n} \ldots z_{i_{k+2}} z_{i_k + i_{k+1} + 1} z_{i_{k-1}} \ldots z_{i_1}) \Bigg). \end{aligned}$$

Next, consider the sum $\sum_{i=1}^{k} \mathrm{I}^{\mathfrak{m}}(n_1, \ldots, n_i + 1, \ldots, n_k)$. We can similarly show that this is equal to

$$\frac{(-1)^N}{2}\Bigg(\mathrm{I}^{\mathfrak{m}}(z_{i_n}\dots z_{i_1}z_1)$$

$$+\sum_{\substack{1<k\leq n\\ i_1+\cdots i_k\equiv k \pmod 2}} \mathrm{I}^{\mathfrak{m}}(z_{i_n}\dots z_{i_{k+1}}z_1z_k\dots z_{i_1})$$

$$-\sum_{\substack{1<k\leq n\\ i_1+\cdots i_k\equiv k+1 \pmod 2}} \mathrm{I}^{\mathfrak{m}}(z_{i_n}\dots z_{i_{k+2}}z_{i_k+i_{k+1}+1}z_{i_{k-1}}\dots z_{i_1})\Bigg).$$

Combining these three equalities, and dividing through by $\frac{(-1)^N}{2}$, we obtain

$$\sum_{k=0}^{n}\mathrm{I}^{\mathfrak{m}}(z_{i_n}\dots z_{i_{k+1}}z_1z_{i_k}\dots z_{i_1})-\sum_{k=1}^{n-1}\mathrm{I}^{\mathfrak{m}}(z_{i_n}\dots,z_{i_{k+2}}z_{i_k+i_{k+1}+1}z_{i_{k-1}}\dots z_{i_1})=0$$

which is precisely that $\mathrm{I}^{\mathfrak{m}}(z_1\,\hat{\sqcup\!\sqcup}\,z_{i_n}\dots z_{i_1})=0$. □

Remark 4.0.8. Note that this is a genuine relation among motivic iterated integrals, not just modulo products. However, as in Lemma 3.1.1, this proof can be identically extended when we consider these motivic iterated integrals modulo products, to obtain that $\mathrm{I}^{\mathfrak{m}}(z_1\,\hat{\sqcup\!\sqcup}\,z_{i_1}\dots z_{i_n})=0$ modulo products, for all $z_{i_1}\dots z_{i_n}\notin\{z_1^{n-1}z_2,\ z_2z_1^{n-1}\}$. Associativity of this quasi-shuffle product then suggests Conjecture 4.0.3 could be strengthened to assume $\mathrm{I}^{\mathfrak{m}}(u\,\hat{\sqcup\!\sqcup}\,v)=0$ modulo products for all $\{u,v\}\not\subset\{z_1^m, z_1^nz_2, z_2z_1^n\}$.

We make the following conjecture, based on numerical evidence, to somehow 'block regularise' $\mathfrak{g}^{\mathfrak{m}}$.

Conjecture 4.0.9. Given $\sigma\in\mathbb{Q}\langle Z\rangle$ of weight n, define $\sigma^*:=\frac{-c_\sigma}{n}(z_1^nz_2-z_2z_1^n)$, where c_σ is the coefficient of z_1z_{n+1} in σ. Then, for all $\sigma\in\mathfrak{g}^{\mathfrak{m}}$, $\sigma+\sigma^*$ is primitive with respect to $\Delta_{\mathfrak{bl}}$.

This regularisation is well defined.

Lemma 4.0.10. *For any* $\sigma,\ \psi\in\mathfrak{g}^{\mathfrak{m}}$

$$\{\sigma+\sigma^*,\psi+\psi^*\}=\{\sigma,\psi\}+\{\sigma,\psi\}^*.$$

Proof. The statement is equivalent to showing

$$\{\sigma, \psi\}^* = \{\sigma, \psi^*\} + \{\sigma^*, \psi\} + \{\sigma^*, \psi^*\}.$$

As, for any element of $\mathfrak{g}^{\mathfrak{m}}$ 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 σ 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 σ is homogeneous of block degree $m-1$ without loss of generality. Switching to the language of commutative polynomials and supposing σ 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. □

Remark 4.0.11. Hirose and Sato claim to have shown 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 4.0.9.

4.1 The block shuffle algebra

Assuming Conjecture 4.0.9, or taking any regularisation procedure, we can use the block shuffle relation to gain further information about both $\mathfrak{g}^{\mathfrak{m}}$, and the Lie coalgebra of motivic multiple zeta values $\mathcal{L}$.

As $\mathfrak{g}^{\mathfrak{m}}$, or rather a regularised $\mathfrak{g}^{\mathfrak{m}}$, is primitive with respect to $\Delta_{\mathfrak{bl}}$, there exists a map $\mathfrak{g}^{\mathfrak{m}} \to \mathcal{P}(Z)$, to the set of primitive elements of $\mathbb{Q}\langle Z\rangle$. We will provide an explicit generating set for Lie algebra $\mathcal{P}(Z)$.

Proposition 4.1.1. *With respect to the coproduct given in Definition 4.0.4,*

$$w_n := \sum_{k\geq 0} \frac{1}{2k+1} \sum_{\substack{i_1+\ldots+i_{2k+1}=n \\ 0<i_j}} z_{i_1}\ldots z_{i_{2k+1}}$$

is primitive.

Proof. We first write $\Delta_{\mathfrak{bl}}(w_n) = \sum_{r,\ s\geq 0} w_{r,s}$, where

$$w_{r,s} \in \mathrm{Span}\{z_{i_1}\ldots z_{i_r} \otimes z_{j_1}\ldots z_{j_s}\ |i_k, j_l \geq 0\}$$

is the degree (r, s) component. As $\Delta_{\mathfrak{bl}}$ is cocommutative, to show w_n is primitive, it suffices to show that $w_{r,s} = 0$ for all $0 < r \leq s$.

Let us consider the contribution of $\Delta_{\mathfrak{bl}}(z_{i_1}\ldots z_{i_{2k+1}})$ to $w_{r,s}$. Every term in this contribution can be identified with a triplet $(\mathbf{j}, C, d)$, consisting of a sequence of integers $0 < j_1 < \cdots < j_m \leq 2k+1$, a composition $C = (c_1, \ldots, c_m)$ of r into m parts, and a sequence $d = \{d_i\} \in \{\pm 1\}^m$, such that

$$2k+1-m+r+\sum_{i=1}^{m} d_i = s.$$

The sequence $\mathbf{j}$ determines which of $z_{i_1}, \ldots, z_{i_{2k+1}}$ contribute terms to the left hand side of the tensor products in $w_{r,s}$. C determines the degree contributed, and d determines the degree contributed to the right hand side. Specifically, $(\mathbf{j}, C, d)$ determines the product

$$Z_{(\mathbf{j},C,d)} := \left(\prod_{u=1}^{j_1-1}(1\otimes z_{i_u})\right)\left(\prod_{t=1}^{m}\left(\sum_{p_1+\cdots+p_{2c_t+d_t}=i_{j_t}} z_{p_1}\dots z_{p_{c_t}}\otimes z_{p_{c_t+1}}\dots z_{p_{2c_t+d_t}}\prod_{v=j_t+1}^{j_{t+1}-1}(1\otimes z_{i_v})\right)\right).$$

Here we take $j_{m+1} = 2k+2$. The sign of this is uniquely determined by (C, d) to be $\prod_{i=1}^m d_i(-1)^{c_i} = (-1)^r \prod_{i=1}^m d_i$.

Letting $\mathcal{C}(r, m)$ be the set of compositions of r into m parts, we can write $w_{r,s}$ as the sum

$$w_{r,s} = \sum_{k\geq 1}\frac{1}{2k+1}\sum_{m=1}^{r}\sum_{\substack{i_1+\cdots i_{2k+1}=n\\ 0<j_1<\cdots<j_m\leq 2k+1}}\sum_{C\in\mathcal{C}(r,m)}\sum_{d\in\{\pm1\}^m}{}' (-1)^r\left(\prod_{t=1}^m d_t\right)Z_{(\mathbf{j},C,d)}$$

where the final sum is restricted to those d such that $2k+1-m+r+\sum_{i=1}^m d_i = s$. Changing this to a restriction on the sum over k, we find

$$w_{r,s} = \sum_{m=1}^{r}\sum_{C\in\mathcal{C}(r,m)}\sum_{d\in\{\pm1\}^m}(-1)^r\left(\prod_{t=1}^m d_t\right)\frac{1}{s+m-r-\sum_{t=1}^m d_t}\sum_{\substack{i_1+\cdots i_{2k+1}=n\\ 0<j_1<\cdots<j_m\leq 2k+1}} Z_{(\mathbf{j},C,d)}.$$

Performing the sums over the i and j indices, we obtain

$$w_{r,s} = \sum_{m=1}^{r}\sum_{C\in\mathcal{C}(r,m)}\sum_{d\in\{\pm1\}^m}(-1)^r\left(\prod_{t=1}^m d_t\right)\frac{1}{s+m-r-\sum_{t=1}^m d_t}\binom{s+m-r-\sum_{t=1}^m d_t}{m}$$
$$\times\sum_{a_1+\cdots+a_{r+s}=n} z_{a_1}\dots z_{a_r}\otimes z_{a_{r+1}}\dots z_{a_{r+s}}.$$

Hence, it suffices to compute

$$\sum_{m=1}^{r}\sum_{C\in\mathcal{C}(r,m)}\sum_{d\in\{\pm1\}^m}\left(\prod_{t=1}^m d_t\right)\frac{1}{s+m-r-\sum_{t=1}^m d_t}\binom{s+m-r-\sum_{i=1}^m d_t}{m}.$$

Note that if $\sum_{t=1}^m d_t = m-q$, then $\prod_{t=1}^m d_t = (-1)^q$, and so we can replace the sum over $d \in \{\pm1\}^m$ 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. □

With this choice of w_n, we can then generate all primitive elements.

Proposition 4.1.2. *The Lie algebra of primitives in* $\mathbb{Q}\langle Z\rangle$ *with respect to* $\Delta_{\mathfrak{bl}}$ *is equal to* *Lie*$[w_1, \ldots, w_n, \ldots]$.

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 $\partial(z_n) = z_n \otimes 1 + 1 \otimes z_n$, and hence $\bar{\sigma} \in \text{Lie}[Z]$. Denote by $\Phi\bar{\sigma}$ the image of $\bar{\sigma}$ under the map

$$\begin{aligned} \text{Lie}[Z] &\to \text{Lie}[w_1, \ldots, w_n, \ldots] \\ z_n &\mapsto w_n \end{aligned}$$

Then $\sigma - \Phi\bar{\sigma}$ is of strictly higher block degree than σ. As block degree is bounded above by weight, we can iterate this process to obtain a finite sequence of elements $\sigma_1, \ldots, \sigma_m \in \text{Lie}[w_1, \ldots, w_n, \ldots]$ such that $\sigma = \sum_{i=1}^{m} \sigma_i \in \text{Lie}[w_1, \ldots, w_n, \ldots]$. □

Remark 4.1.3. The work of Hirose and Sato, along side Proposition 4.1.2, suggests the existence of an injection $\mathfrak{g}^{\mathfrak{m}} \to \text{Lie}[w_1, \ldots, w_n, \ldots]$. However the following diagram does not commute.

$$\begin{tikzcd}
\mathfrak{g}^{\mathfrak{m}} \arrow[r, hook] \arrow[d] & \mathrm{Lie}[w_1, \ldots, w_n, \ldots] \\
\mathfrak{bg} \arrow[r, hook] & \mathrm{Lie}[z_1, \ldots, z_n, \ldots] \arrow[u, "z_n \mapsto w_n"']
\end{tikzcd}$$

If we could choose an automorphism of $\mathrm{Lie}[w_1, \ldots, w_n, \ldots]$ mapping $\{w_n\}_{n\geq 1}$ to another set of generators$\{w'_n\}_{n\geq 1}$, such that the composition

$$\mathfrak{bg} \hookrightarrow \mathrm{Lie}[z_1, \ldots, z_n, \ldots] \xhookrightarrow{z_n \mapsto w'_n} \mathrm{Lie}[w'_1, \ldots, w'_n, \ldots]$$

maps $\mathfrak{bg}$ to the image of $\mathfrak{g}^{\mathfrak{m}}$, we could use this to define canonical σ_{2k+1}.

Dualising the map in Proposition 4.1.2, we will obtain an isomorphism between the shuffle algebra $(\mathbb{Q}\langle Z\rangle, \shuffle)$, and the block shuffle algebra $(\mathbb{Q}\langle Z\rangle, \hat{\shuffle})$, which can be used to produce relations in $\mathcal{L}$, analogously to Hoffman's work on quasishuffle algebras [32], [30]. 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 4.1.4. A composition I of n is a sequence of positive integers $(i_1, \ldots, i_l)$ such that $i_1 + \cdots i_l = n$. Given a composition I of n into l parts and a composition J of l into k parts, we define the product composition:

$$J \circ I := (i_1 + \cdots i_{j_1}, i_{j_1+1} + \cdots + i_{j_1+j_2}, \ldots, i_{j_1+\cdots+j_{k-1}+1} + \cdots + i_{j_1+\cdots+j_k}).$$

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 $[z_{a_1} \ldots z_{a_k}] := z_{a_1+\cdots+a_k}$, and given a compositon I of n, define

$$I[z_{a_1} \ldots z_{a_n}] := [z_{a_1} \ldots z_{a_{i_1}}][z_{a_{i_1}+1} \ldots z_{a_{i_1+i_2}}] \cdots [z_{a_{i_1+\cdots+i_{l-1}+1}} \ldots z_{a_n}]$$

and $I[w] = 0$ for any words not of length n.

Proposition 4.1.5. *Let $Tanh : \mathbb{Q}\langle Z\rangle \to \mathbb{Q}\langle Z\rangle$ be the linear map with $Tanh(1) = 1$ and,* *for w a word of length n*

$$Tanh(w) = \sum_{(i_1,\ldots,i_l)\in\mathcal{C}(n)} c_{i_1}\ldots c_{i_l}(i_1,\ldots,i_l)[w]$$

where c_j is the coefficient of x^j in the Taylor expansion of $tanh(x)$. Then Tanh is an algebra isomorphism

$$Tanh : (\mathbb{Q}\langle Z\rangle, ⧢) \to (\mathbb{Q}\langle Z\rangle, \hat{⧢}).$$

To prove this, we require the following two lemmas. The first is due to Hoffman [32].

Lemma 4.1.6. *Let $f(z) = c_1z + c_2z^2 + \cdots$ be a function analytic at 0, with $c_1 \neq 0$, and $c_i \in \mathbb{Q}$ for all i. Let $f^{-1}(z) = b_1z + b_2z^2 + \cdots$ be its inverse. Then the map $\Psi_f : \mathbb{Q}\langle Z\rangle \to \mathbb{Q}\langle Z\rangle$ given by*

$$\Psi_f(w) = \sum_{(i_1,\ldots,i_l)\in\mathcal{C}(n)} c_{i_1}\ldots c_{i_l}(i_1,\ldots,i_l)[w]$$

for words of length n, and extended linearly to $\mathbb{Q}\langle Z\rangle$, has inverse $\Psi_f^{-1} = \Psi_{f^{-1}}$.

We use this lemma to establish Tanh as the inverse map of a homomorphism Tanh^{-1} given by the dual of the coalgebra homomorphism $z_n \mapsto w_n$, hence avoiding having to establish that Tanh is a homomorphism directly.

Lemma 4.1.7. *The dual of $\Phi : (\mathbb{Q}\langle Z\rangle, \Delta) \to (\mathbb{Q}\langle Z\rangle, \Delta_{\mathfrak{bl}})$, $\Phi(z_n) := w_n$ is given by $\Psi_{tanh^{-1}}$, and defines a homomorphism $Tanh^{-1} : (\mathbb{Q}\langle Z\rangle, \hat{⧢}) \to (\mathbb{Q}\langle Z\rangle, ⧢)$.*

Proof. As a consequence of Proposition 4.1.1, Φ is a coalgebra homomorphism, and hence its dual will define an algebra homomorphism. Hence, it is sufficient to show that $\Phi^* = \Psi_{tanh^{-1}}$. 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

$$\begin{aligned}\langle \Phi^*(w), z_{a_1}\dots z_{a_l}\rangle &= \langle w, \Phi(z_{a_1}\dots z_{a_n})\rangle \\ &= \langle w, \prod_{i=1}^{l} \sum_{1\le 2k_i+1\le a_i} \frac{1}{2k_i+1} \sum_{i_1+\ldots+i_{2k_i+1}=a_i} z_{i_1}\dots z_{i_{2k_i+1}}\rangle,\end{aligned}$$

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

$$\Phi^*(w) = \sum_{\substack{(i_1,\ldots,i_l)\in\mathcal{C}(n)\\ i_j \text{ odd}}} \frac{1}{i_1\dots i_l}(i_1,\dots,i_l)[w]$$

which is precisely $\Psi_{tanh^{-1}}$. The result then follows. $\square$

As a corollary to Proposition 4.1.5, we obtain the following.

Corollary 4.1.8. $(\mathbb{Q}\langle Z\rangle, \widehat{\sqcup\!\sqcup})$ *is the free polynomial algebra on the Lyndon words.*

Proof. Hoffman's proof of Theorem 2.6 [32] applies exactly. We sketch the proof here, but refer the reader to Hoffman's proof for further detail. The proof proceeds by induction on the length of a word. Suppose w is a word of length l. As $(\mathbb{Q}\langle Z\rangle, \sqcup\!\sqcup)$ is a free polynomial algebra on Lyndon words, there exist Lyndon words $w_1,\dots,w_n$ and a polynomial P such that

$$w = P(\mathrm{Tanh}(w_1), \mathrm{Tanh}(w_2), \dots, \mathrm{Tanh}(w_n))$$

where P is considered as a $\widehat{\sqcup\!\sqcup}$-polynomial. Since the shuffle product preserves length, and $\mathrm{Tanh}^{-1}(w)$ has terms with length at most l, we can assume every term of $P(w_1,\dots,w_n)$ has length at most l, where P is considered as a $\sqcup\!\sqcup$-polynomial. But then

$$w - P(w_1,\dots,w_n) = P(\mathrm{Tanh}(w_1),\dots,\mathrm{Tanh}(w_n)) - P(w_1,\dots,w_n)$$

has only terms of length less than l, and so can be written as a $\widehat{\sqcup\!\sqcup}$-polynomial of Lyndon words. $\square$

Corollary 4.1.9. *Recall we have a surjective linear map* $I^{\mathfrak{l}} : \mathbb{Q}\langle Z\rangle \to \mathcal{L}$, *mapping a word to its corresponding iterated integral modulo products. Denote by* $L(Z)$ *the* $\mathbb{Q}$*-span of the* *set of Lyndon words in Z. Then $\mathcal{L} = I^{\mathfrak{t}}(L(Z))$.*

Proof. Every word in $\mathbb{Q}\langle Z\rangle$ can be written as a $\widehat{\shuffle}$-polynomial in the Lyndon words. Proposition 4.0.3 tells us that the image of any terms of degree greater than 1 in this polynomial is 0, and hence $\mathrm{I}^{\mathfrak{t}}(w)$ is the image of the linear part, i.e. $\mathrm{I}^{\mathfrak{t}}(w) \in \mathrm{I}^{\mathfrak{t}}(L(Z))$. □

4.2 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 [30]. We first recall one of their results, specialised to the case of block shuffle. In all that follows, λ is a formal parameter, and we extend Ψ_f by $\Psi_f(\lambda) = \lambda$.

Definition 4.2.1. Define $\lozenge : \mathbb{Q}Z \otimes \mathbb{Q}Z \to \mathbb{Q}Z$ by $z_m \lozenge z_n := z_{m+n}$. Then, for any $f(z) = c_1 z + c_2 z^2 + \cdots$, define

$$f_\bullet(\lambda w) := \sum_{i=1}^{\infty} \lambda^i c_i w^{\bullet i}$$

for $\bullet \in \{\shuffle, \widehat{\shuffle}\}$ and $w \in \mathbb{Q}\langle Z\rangle$, or $\bullet = \lozenge$ and $w \in \mathbb{Q}Z$.

Remark 4.2.2. 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 4.2.3 (Theorem 5.1 [30])**.** *For any $f(z) = c_1 z + c_2 z^2 + \cdots$ and $z \in \mathbb{Q}Z[[\lambda]]$,*

$$\Psi_f\left(\frac{1}{1-\lambda z}\right) = \frac{1}{1 - f_\lozenge(\lambda z)}.$$

We also need a modification of a lemma due to Hoffman and Ihara.

Lemma 4.2.4. *For $z \in \mathbb{Q}Z[[\lambda]]$*

$$exp_{\widehat{\shuffle}}(\lambda z) = Tanh\left(\frac{1}{1-\lambda z}\right).$$

Proof. Since $\mathrm{Tanh} : (\mathbb{Q}\langle Z\rangle, \shuffle) \to (\mathbb{Q}\langle Z\rangle, \hat{\shuffle})$ is an algebra isomorphism, we must have that $\mathrm{Tanh} \circ f_{\shuffle} = f_{\hat{\shuffle}} \circ \mathrm{Tanh}$. Thus, as $\mathrm{Tanh}|_{\mathbb{Q}Z} = id$, we have

$$exp_{\hat{\shuffle}}(\lambda z) = exp_{\hat{\shuffle}}(\mathrm{Tanh}(\lambda z)) = \mathrm{Tanh}(exp_{\shuffle}(\lambda z)) = \mathrm{Tanh}\left(\frac{1}{1-\lambda z}\right)$$

where we have used that

$$exp_{\shuffle}(\lambda z) = \sum_{n=0}^{\infty} \lambda^n \frac{z^{\shuffle n}}{n!} = \sum_{n=0}^{\infty} \lambda^n \frac{n! z^n}{n!} = \sum_{n=0}^{\infty} \lambda^n z^n.$$

□

Thus we can show the following

Proposition 4.2.5. *For* $z \in \mathbb{Q}A[[\lambda]]$

$$exp_{\hat{\shuffle}}(tanh_{\lozenge}^{-1}(1+\lambda z)) = \frac{1}{1-\lambda z}.$$

Proof. By Lemma 4.2.4, this is equivalent to showing that

$$\mathrm{Tanh}\left(\frac{1}{1 - tanh_{\lozenge}^{-1}(1+\lambda z)}\right) = \frac{1}{1-\lambda z}.$$

However, this follows immediately from the statement of Proposition 4.2.3 for $f = tanh^{-1}$.

□

Corollary 4.2.6. *For any* $z \in \mathbb{Q}Z$ *and any* $n > 1$, $I^{\mathfrak{t}}(z^n) = 0$.

Proof. Taking the image of the equality in Proposition 4.2.5, we obtain

$$\mathrm{I}^{\mathfrak{t}}(1 + tanh_{\lozenge}^{-1}(1+\lambda z) + \sum_{n\geq 2} \frac{tanh_{\lozenge}^{-1}(\lambda z)^{\hat{\shuffle} n}}{n!}) = \sum_{n\geq 0} \lambda^n \mathrm{I}^{\mathfrak{t}}(z^n).$$

As $\mathrm{I}^{\mathfrak{t}}$ kills $\hat{\shuffle}$-products, the left hand side is just $\lambda \mathrm{I}^{\mathfrak{t}}(z)$. Comparing coefficients of λ^n, we see that $\mathrm{I}^{\mathfrak{t}}(z^n) = 0$ for all $n > 1$. □

Remark 4.2.7. As $\mathrm{I}^{\mathfrak{t}}(w) = 0$ if the length of w and the weight of w are of the same parity, we see that the projection of z onto $\bigoplus_{i=1}^{\infty} \mathbb{Q}z_{2i}$ must be non-zero for the statement to be non-trivial. Additionally, as $\mathrm{I}^{\mathfrak{t}}(w) = (-1)^{|w|}\mathrm{I}^{\mathfrak{t}}(Dw)$, and $(z_{i_1} + \cdots + z_{i_k})^n = D(z_{i_1} + \cdots + z_{i_k})$, we obtain a trivial statement in odd weight. Hence we must take $z \in \bigoplus_{i=1}^{\infty} \mathbb{Q} z_{2i}$ and n odd to obtain something interesting.

Example 4.2.8. Consider $z = z_2$, then $\mathrm{I}^{\mathfrak{l}}(z_2^{2k+1})$ is the image of $\zeta^{\mathfrak{a}}(\{1,3\}^k)$ in $\mathcal{L}$, and thus $\zeta^{\mathfrak{a}}(\{1,3\}^k) = 0$ mod products. It is known due the work of Borwen, Bradley, Broadhurst, and Lisonek [6] that we in fact have $\zeta(\{1,3\}^k) = \frac{2\pi^{4k}}{(4k+2)!}$. Similarly, Theorem 2 of [6] tells us that $\zeta(2 ⧢ \{1,3\}^n) = \frac{\pi^{4n+2}}{(4n+3)!}$ and taking $z = z_2 + z_4$, and considering the weight $4n+2$ part of z^{2n+1}, we see that $\zeta^{\mathfrak{a}}(2 ⧢ \{1,3\}^n) = 0$ mod products.

We can generalise this by considering the weight $4n + 2k$ part of z^{2n+1} for $z = z_2 + z_4 + \cdots + z_{2k+2}$, we obtain $\zeta^{\mathfrak{a}}(\{2\}^k ⧢ \{1,3\}^n) = 0$ modulo products. We conjecture that the numerical sums evaluate to rational multiples of π^{4n+2k}. The cases $k = 0$, and $k = 1$ have been discussed. Checking the first few values numerically for $k = 2, 3, \ldots, 7$ [5], we make the following more precise conjecture, which we will prove in Theorem 4.3.14.

Conjecture 4.2.9.

$$\zeta(\{2\}^k ⧢ \{1,3\}^n) = \frac{\pi^{4n+2k}}{(2n+1)(4n+2k+1)!}\binom{2n+k}{k}$$

for all non-negative n, k.

Considering other weights, taking z to be some other linear combination, we obtain that sums over certain subsets of the set of shuffles also evaluate to 0 modulo products.

Proposition 4.2.10. *Let $S_{n,k,p}$ denote the set of words in $\{1,2,3\}$ appearing in the shuffle product $\{2\}^k ⧢ \{1,3\}^n$ containing at least one group of p adjacent 2s, and no group of $p+1$ adjacent 2s. Then*

$$\sum_{u \in S_{n,k,p}} \zeta^{\mathfrak{a}}(u) = 0 \text{ modulo products.}$$

Proof. Corollary 4.2.6 tells us that, for any $n, p \geq 1$

$$\mathrm{I}^{\mathfrak{l}}((z_2 + \cdots + z_{2p+2})^{2n+1}) = 0$$

Considering the difference of two such equalities, we see that

$$\mathrm{I}^{\mathfrak{l}}(((z_2 + \cdots + z_{2p+2})^{2n+1} - (z_2 + \cdots + z_{2p})^{2n+1})) = 0.$$

Letting $T_{n,k,p}$ be the set of all monomials of block degree $2n$, weight $4n+2k$, containing at least one z_{2p+2}, this is precisely the statement that

$$\sum_{w \in T_{n,k,p}} \mathrm{I}^{\mathfrak{l}}(w) = 0.$$

Translating this into the language of motivic multiple zeta values, we note that every z_{2k+2} corresponds to a group of exactly k adjacent 2s, and so elements of $T_{n,k,p}$ correspond exactly to elements of $S_{n,k,p}$. The result then follows. □

Example 4.2.11. For example, if we take $z = z_4$, we obtain that $\zeta^{\mathfrak{a}}(\{2,1,2,3\}^k, 2) = 0$ modulo products. This corresponds to $S_{k,k+1,1}$. Checking the first few values of this numerically [5], we conjecture that $\zeta^{\mathfrak{a}}(\{2,1,2,3\}^k, 2) = \frac{\pi^{8k+2}}{(2k+1)(8k+3)!} = \frac{4\pi^{8k+2}}{(8k+4)!}$. It would be interesting to see if every such sum evaluates to a rational multiple of a power of π.

Remark 4.2.12. We can actually refine this result significantly: by considering $z := a_2 z_2 + \cdots + a_{2p+2} z_{2p+2}$, and allowing the a_{2i} to vary freely, we see that we must have

$$\sum_{u \in I_{i_1,\ldots,i_{p+1},n,w}} \mathrm{I}^{\mathfrak{l}}(u) = 0$$

where $I_{i_1,\ldots,i_{p+1},n,w}$ is the set of words of degree $2n+1$ and weight w with $\deg_{z_{2j}}(u) = i_j$. This implies

$$\sum_{(n_1,\ldots,n_k) \in J_{i_1,\ldots,i_{p+1},n,w}} \zeta^{\mathfrak{a}}(n_1,\ldots,n_k) = 0 \text{ modulo products}$$

where $J_{i_1,\ldots,i_{p+1},n,w}$ is the set of tuples $(n_1,\ldots,n_k)$ with $n_i \in \{1,2,3\}$, exactly n of which are 1 and exactly n of which are three such that $n_1+\cdots+n_k = w$ and $(n_1,\ldots,n_k)$ contains exactly i_j groups of exactly $j-1$ adjacent 2s, for $j > 1$.

Numerical evidence suggests that every such sum is a rational multiple of π^w.

4.3 Genuine relations among motivic multiple zeta values

Given a relation among motivic multiple zeta values modulo products, there is the obvious question of what the product terms are. While this is in general quite a challenging problem, we can approach this modulo $\zeta^{\mathfrak{m}}(2)$ in block degrees 1 and 2.

We first note that block graded relations in block degree 1 and 2 are genuine relations modulo products. Recall Lemma 2.1.10 tells us that we must have $\deg_{\mathcal{B}}(w) \cong |w| \bmod 2$. Hence, we cannot have relations among terms of block degree 1 and block degree 0. In particular, relations among motivic iterated integrals of block degree 1 modulo terms of lower block degree are genuine relations modulo products. Similarly, as $\mathcal{B}_0\mathcal{H} = (\zeta^{\mathfrak{m}}(2))$, we have that relations among motivic iterated integrals of block degree 2 modulo terms of lower block degree are genuine relations modulo products.

Relations in block degree 1 are completely described by duality, shuffle regularisation, and Zagier's formula [42][9]

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

Relations in block degree 2 are much more interesting. We will consider block shuffle and the relations arising from dihedral symmetry. To compute the products, we follow the decomposition procedure outlined by Brown [22]. This algorithm allows us to present a weight N relation in a chosen algebra basis, up to a multiple of $\zeta^{\mathfrak{m}}(N)$. As we work modulo $\zeta^{\mathfrak{m}}(2)$, and block degree 2 is necessarily of even weight, we obtain an exact decomposition.

We first recall a few key points from Brown's work [9].

Definition 4.3.1. Define $\partial_{2k+1} : \mathcal{H} \to \mathcal{H}$ by $\partial_{2k+1} := (c_{2k+1} \otimes \mathrm{id}) \circ D_{2k+1}$. Here c_{2k+1} extracts the coefficient of $\zeta^{\mathfrak{m}}(2k+1)$ in the left hand term.

Proposition 4.3.2 (Brown)**.** *The coefficient of $\zeta^{\mathfrak{m}}(2r+1)\zeta^{\mathfrak{m}}(2s+1)\zeta^{\mathfrak{m}}(2)^n$ in the decomposition of $\zeta^{\mathfrak{m}}(w)$ into the algebra basis containing $\zeta^{\mathfrak{m}}(2k+1)$ for every $k \geq 1$ is given by $c_2^n\partial_{2s+1}\partial_{2r+1}$, where c_2^n means taking the coefficient of $\zeta^{\mathfrak{m}}(2)^n$.*

Note that, as we work in block degree 2, and each ∂_{2k+1} reduces the block degree by one, as in Proposition 2.1.7, we need only consider composition of two delta operators. Working modulo $\zeta^{\mathfrak{m}}(2)$, it therefore is sufficient to consider $\partial_{2s+1}\partial_{2r+1}$ where $2r + 2s + 2$ is equal to the weight.

Lemma 4.3.3.

$$\partial_{2k+1}(I^{\mathfrak{m}}(x_a x_b)) = \sum_{i=1}^{2k+2} c^{2k+1}_{2k+3-i,i} I^{\mathfrak{m}}(x_{a+b-2k-1}) \mathbb{1}_{\substack{a \geq 2r+3-i, \\ b \geq i}}$$

$$\partial_{2k+1}(I^{\mathfrak{m}}(x_a x_b x_c)) = \sum_{i=1}^{2k+2} c^{2k+1}_{2k+3-i,i} \left(I^{\mathfrak{m}}(x_{a+b-2k-1} x_c) \mathbb{1}_{\substack{a \geq 2k+3-i \\ b \geq i}} + I^{\mathfrak{m}}(x_a x_{b+c-2k-1}) \mathbb{1}_{\substack{b \geq 2k+3-i \\ c \geq i}} \right),$$

$$\partial_{2k+1}(I^{\mathfrak{m}}(x_{a_1} \dots x_{a_n})) = \sum_{i=1}^{2k+2} \sum_{j=1}^{n-1} c^{2k+1}_{2k+3-i,i} I^{\mathfrak{m}}(x_{a_1} \dots x_{a_{j-1}} x_{a_j + a_{j+1} - 2k-1} x_{a_{j+2}} \dots x_{a_n}) \mathbb{1}_{\substack{a_j \geq 2k+3-i, \\ a_{j+1} \geq i}}$$

where $\frac{c^{2k+1}_{i,j}}{2(-1)^k}$ *is the coefficient of* $x_1^i x_2^j$ *in* $p_{2k+1}(x_1, x_2)$ *and* $\mathbb{1}_P$ *is the indicator function for a logical statement* P*.*

Proof. We will demonstrate the proof in the first case, as the argument generalises easily. First note that, following Zagier's result, we see that the coefficient of $\zeta^{\mathfrak{m}}(2k+1)$ in $\mathrm{I}^{\mathfrak{m}}(x_{2a+1} x_{2b+2})$ is given by $c^{2k+1}_{2a+1,2b+2}$ if $a + b = k$. Similarly, the coefficient of $\zeta^{\mathfrak{m}}(2k+1)$ in $\mathrm{I}^{\mathfrak{m}}(x_{2a+2} x_{2b+1})$ is given by $c^{2k+1}_{2a+2,2b+1}$ if $a + b = k$. Now, consider $\partial_{2k+1}(\mathrm{I}^{\mathfrak{m}}(x_a x_b))$. We may assume, without loss of generality, that $a = 2s+1$ is odd and $b = 2t+2$ is even. Then

$$\mathrm{I}^{\mathfrak{m}}(x_a x_b) = \mathrm{I}^{\mathfrak{m}}(0; \{1,0\}^s, 0, \{1,0\}^t; 1).$$

Considering D_{2k+1} of this, the only non zero terms are those in the sum

$$\sum_{i=0}^{k} \mathbb{1}_{\substack{2s+1 \geq 2k+1-2i \\ 2t \geq 2i}} \mathrm{I}^{\mathfrak{l}}(0; \{1,0\}^{k-i}, 0, \{1,0\}^i; 1) \otimes \mathrm{I}^{\mathfrak{m}}(0; \{1,0\}^{s+t-k}; 1)$$
$$+ \sum_{i=0}^{k} \mathbb{1}_{\substack{2s \geq 2k+2-2i \\ 2t \geq 2i}} \mathrm{I}^{\mathfrak{l}}(1; \{0,1\}^{k-i}, 0, \{0,1\}^i; 0) \otimes \mathrm{I}^{\mathfrak{m}}(0; \{1,0\}^{s+t-k}; 1).$$

Thus, as $\mathrm{I}^{\mathfrak{l}}(1; \{0,1\}^{k-i}, 0, \{0,1\}^i; 0) = -\mathrm{I}^{\mathfrak{l}}(0; \{1,0\}^i, 0, \{1,0\}^{k-i}; 1)$, we obtain that the non-zero part is the sum

$$\sum_{i=0}^{k} \mathbb{1}_{\substack{2s+1 \geq 2k+1-2i \\ 2t \geq 2i}} \mathrm{I}^{\mathfrak{l}}(x_{2k+1-2i} x_{2i+2}) \otimes \mathrm{I}^{\mathfrak{m}}(x_{2s+2t+2-2k})$$
$$- \sum_{i=0}^{k} \mathbb{1}_{\substack{2s \geq 2k+2-2i \\ 2t \geq 2i}} \mathrm{I}^{\mathfrak{l}}(x_{2i+1} x_{2k-2i+2}) \otimes \mathrm{I}^{\mathfrak{m}}(x_{2s+2t+2-2k}).$$

Letting $i \mapsto k+1-i$ in the second sum, and using $\mathrm{I}^{\mathfrak{l}}(x_m x_n) = -\mathrm{I}^{\mathfrak{l}}(x_n x_m)$, this reduces to

$$\sum_{i=1}^{2k+2} \mathbb{1}_{\substack{2s+1 \geq 2k+3-2i \\ 2t+2 \geq 2i}} \mathrm{I}^{\mathfrak{l}}(x_{2k+3-2i} x_i) \otimes \mathrm{I}^{\mathfrak{m}}(x_{2s+2t+2-2k}).$$

Applying the map $c_{2k+1} \otimes \mathrm{id}$ gives the desired result. The other cases follow similarly. □

Proposition 4.3.4. *Modulo $\zeta^{\mathfrak{m}}(2)$, we have*

$$I^{\mathfrak{m}}(x_a x_b x_c) + I^{\mathfrak{m}}(x_b x_a x_c) + I^{\mathfrak{m}}(x_b x_c x_a) = 0.$$

Proof. It suffices to show

$$\partial_{2s+1}\partial_{2r+1}(\mathrm{I}^{\mathfrak{m}}(x_a x_b x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_a x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_c x_a)) = 0$$

for $2r+2s+4 = a+b+c$. It is an easy computation using Lemma 4.3.3 to show

$$\begin{aligned}
&\partial_{2s+1}\partial_{2r+1}(\mathrm{I}^{\mathfrak{m}}(x_a x_b x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_a x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_c x_a)) \\
&= \sum_{i=1}^{2r+2} \Bigg(c^{2r+1}_{2r+3-i,i} c^{2s+1}_{a+b-2r-1,c} \mathbb{1}_{\substack{a \geq 2r+3-i \\ b \geq i}} + c^{2r+1}_{2r+3-i,i} c^{2s+1}_{a,b+c-2r-1} \mathbb{1}_{\substack{b \geq 2r+3-i \\ c \geq i}} \\
&\quad + c^{2r+1}_{2r+3-i,i} c^{2s+1}_{a+b-2r-1,c} \mathbb{1}_{\substack{b \geq 2r+3-i \\ a \geq i}} + c^{2r+1}_{2r+3-i,i} c^{2s+1}_{b,a+c-2r-1} \mathbb{1}_{\substack{a \geq 2r+3-i \\ c \geq i}} \\
&\quad + c^{2r+1}_{2r+3-i,i} c^{2s+1}_{b+c-2r-1,a} \mathbb{1}_{\substack{b \geq 2r+3-i \\ c \geq i}} + c^{2r+1}_{2r+3-i,i} c^{2s+1}_{b,a+c-2r-1} \mathbb{1}_{\substack{c \geq 2r+3-i \\ a \geq i}} \Bigg).
\end{aligned}$$

Then, noting that under the substitution $i \mapsto 2r+3-i$, we have the following equality.

$$\sum_{i=1}^{2r+2} c^{2r+1}_{2r+3-i,i} \mathbb{1}_{\substack{a \geq 2r+3-i \\ b \geq i}} = -\sum_{i=1}^{2r+2} c^{2r+1}_{2r+3-i,i} \mathbb{1}_{\substack{b \geq 2r+3-i \\ a \geq i}}.$$

Recalling also that $c^{2k+1}_{i,j} = -c^{2k+1}_{j,i}$, we see that the above sum vanishes. □

Remark 4.3.5. Note that the vanishing of $\partial_{2s+1}\partial_{2r+1}(\mathrm{I}^{\mathfrak{m}}(x_a x_b x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_a x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_c x_a))$ in the above proof does not require $2r+2s+4 = a+b+c$. Thus we can conclude that

$$\mathrm{I}^{\mathfrak{m}}(x_a x_b x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_a x_c) + \mathrm{I}^{\mathfrak{m}}(x_b x_c x_a) = \alpha \zeta^{\mathfrak{m}}(2)^{\frac{a+b+c-2}{2}}$$

for some rational α.

Lemma 4.3.6. *The cyclic symmetry of* $\mathfrak{rbg}$ *implies*

$$I^{\mathfrak{bl}}(x_{a-1}x_bx_c) + I^{\mathfrak{bl}}(x_{a-1}x_cx_b) = I^{\mathfrak{bl}}(x_ax_{b-1}x_c) + I^{\mathfrak{bl}}(x_ax_{c-1}x_b).$$

Proof. Let $f(x_1, x_2, x_3) = x_1x_2x_3(x_1 - x_3)r(x_1, x_2, x_3) \in \mathfrak{bg}$.Then

$$\begin{aligned}(x_2 - x_1)f(x_1, x_2, x_3) &= x_1x_2x_3(x_1 - x_3)(x_2 - x_1)r(x_1, x_2, x_3)\\ &= x_1x_2x_3(x_1 - x_3)(x_2 - x_1)r(x_2, x_3, x_1)\\ &= (x_1 - x_3)f(x_2, x_3, x_1).\end{aligned}$$

Comparing coefficients of $x_1^a x_2^b x_3^t$ we see that

$$\mathrm{I}^{\mathfrak{bl}}(x_ax_{b-1}x_c) - \mathrm{I}^{\mathfrak{bl}}(x_{a-1}x_cx_b) = \mathrm{I}^{\mathfrak{bl}}(x_bx_cx_{a-1}) - \mathrm{I}^{\mathfrak{bl}}(x_bx_{c-1}x_a)$$

which, upon applying $\mathrm{I}^{\mathfrak{bl}}(x_kx_lx_m) = \mathrm{I}^{\mathfrak{bl}}(x_mx_lx_k)$, rearranges to the desired identity. □

A similar computation to that of Proposition 4.3.4 shows the following

Proposition 4.3.7. *For* $a + b + c = 2N + 3$,

$$\begin{aligned}&I^{\mathfrak{m}}(x_{a-1}x_bx_c) + I^{\mathfrak{m}}(x_{a-1}x_cx_b) - I^{\mathfrak{m}}(x_ax_{b-1}x_c) - I^{\mathfrak{m}}(x_ax_{c-1}x_b)\\ &= \sum_{\substack{s\geq r\\ 2r+2s+2\leq 2N}} \alpha_{r,s}\zeta^{\mathfrak{m}}(2r+1)\zeta^{\mathfrak{m}}(2s+1)\zeta^{\mathfrak{m}}(2)^{N-r-s-1}\end{aligned}$$

up to a rational multiple of $\zeta^{\mathfrak{m}}(2)^N$, *where*

$$\begin{aligned}\alpha_{r,s} = \sum_{j=1}^{2s+2} c^{2s+1}_{2s+3-j,j}\Big[&(c^{2r+1}_{2r+3-a,a} + c^{2r+1}_{2r+3-b,b})\mathbb{1}_{a+b\geq 2r+4}\mathbb{1}_{a+b\geq 2r+2s+5-j}\mathbb{1}_{c\geq j}\\ &+ (c^{2r+1}_{2r+3-a,a} + c^{2r+1}_{2r+3-c,c})\mathbb{1}_{a+c\geq 2r+4}\mathbb{1}_{a+c\geq 2r+2s+5-j}\mathbb{1}_{b\geq j}\Big].\end{aligned}$$

We now return to Conjecture 4.2.9. We prove this analogously to the proof of the $k = 0,\ 1$ cases shown in [6]. We first give several definitions.

Definition 4.3.8. Let p, q, j be non-negative integers such that $j \leq \min(p, q)$, and define $S_{p+q,j}$ to be the set of words occurring in $(ba)^p \shuffle (ba)^q$ containing the subword a^2 exactly j times.

Remark 4.3.9. As noted in [6], the set $S_{p+q,j}$ depends only on $p+q$ so long as $j \leq \min(p,q)$. Note also that we must have equal numbers of subwords a^2 as b^2, and thus $S_{p+q,j}$ contains only words of block degree $2j$. We can similarly conclude $|S_{p+q,j}| = \binom{p+q}{2j}$.

Definition 4.3.10. Let p, q, j be as before. Define $T_{p+q,j} := \sum_{w \in S_{p+q,j}} w$.

Every term in the sum $\{2\}^k ⧢ \{1,3\}^n$ corresponds to a word in $S_{2n+k,n}$, and there are exactly $\binom{2n+k}{2n}$ terms, so we must have that $\zeta(T_{2n+k,n}) = \zeta(\{2\}^k ⧢ \{1,3\}^n)$. So to evaluate the sum in Conjecture 4.2.9, we need only consider the combinatorics of $T_{p+q,j}$.

Proposition 4.3.11 (BBBL [6])**.** *For any non-negative integers p, q, we have*

$$(ba)^p ⧢ (ba)^q = \sum_{j=0}^{min(p,q)} 4^j \binom{p+q-2j}{p-j} T_{p+q,j}.$$

Using this, we can express $T_{2n+k,n}$ in terms of shuffle products. We first require a combinatorial lemma.

Lemma 4.3.12. *For any non-negative integers n, k, we have*

$$\sum_{r=0}^{n} (-1)^r \left(\binom{k+r}{k} + \binom{k+r-1}{k} \right) \binom{2n+k}{n-r} = \delta_{n,0}.$$

Proof. The statement of this theorem is equivalent to the statement that

$$\sum_{n\geq 0} \sum_{r \in \mathbb{Z}} (-1)^r \left(\binom{k+r}{k} + \binom{k+r-1}{k} \right) \binom{2n+k}{n-r} y^n = 1.$$

To evaluate this function, we first consider the function

$$G(x,y) := \sum_{n\geq 0} \sum_{r \in \mathbb{Z}} (-1)^r \left(\binom{k+r}{k} + \binom{k+r-1}{k} \right) \binom{2n+k}{n-r} x^r y^n.$$

Thus, we wish to show that $G(1,y) = 1$. We first recall two standard identities among generating series

$$\sum_{n\geq 0} \binom{2n+k}{n} t^n = \frac{1}{\sqrt{1-4t}} \left(\frac{2}{1+\sqrt{1-4t}} \right)^k,$$

$$\sum_{n\geq 0} \binom{n}{k} t^n = \frac{t^k}{(1-t)^{k+1}}.$$

Using these, we can rewrite $G(x, y)$ as follows.

$$\begin{aligned}
G(x,y) &= \sum_{n\geq 0}\sum_{r\in\mathbb{Z}}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\binom{2n+k}{n-r}x^ry^n\\
&= \sum_{r\in\mathbb{Z}}(-xy)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\sum_{n\geq r}\binom{2n+k}{n-r}y^{n-r}\\
&= \sum_{r\in\mathbb{Z}}(-xy)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\sum_{m\geq 0}\binom{2m+2r+k}{m}y^{m}\\
&= \sum_{r\in\mathbb{Z}}(-xy)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\times\frac{1}{u}\left(\frac{2}{1+u}\right)^{2r+k}\\
&= \frac{1}{u}\left(\frac{2}{1+u}\right)^{k}\sum_{r\in\mathbb{Z}}\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\left(\frac{-4xy}{(1+u)^2}\right)^r,
\end{aligned}$$

where $u := \sqrt{1-4y}$. Let $q := \frac{-4xy}{(1+u)^2}$. We can then evaluate the remaining sum.

$$\begin{aligned}
G &= \frac{1}{u}\left(\frac{2}{1+u}\right)^{k}\sum_{r\in\mathbb{Z}}\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)q^r\\
&= \frac{1}{u}\left(\frac{2}{1+u}\right)^{k}\left(q^{-k}\sum_{m\geq 0}\binom{m}{k}q^m+q^{1-k}\sum m\geq 0\binom{m}{k}q^m\right)\\
&= \frac{1}{u}\left(\frac{2}{1+u}\right)^{k}\left(\frac{1+q}{(1-q)^{k+1}}\right)
\end{aligned}$$

Now, at $x = 1$,

$$q = \frac{-4y}{(1+u)^2} = \frac{u^2-1}{(1+u)^2} = \frac{u-1}{u+1},$$

and so $1-q = \frac{2}{u+1}$ and $1+q = \frac{2u}{u+1}$. Thus, we find

$$G(1,y) = \frac{1}{u}\left(\frac{2}{1+u}\right)^{k}\left(\frac{u+1}{2}\right)^{k+1}\left(\frac{2u}{u+1}\right) = 1.$$

The result then follows. □

Corollary 4.3.13. *For any non-negative integers n, k, we have*

$$\sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)[(ba)^{n-r}\shuffle(ba)^{n+k+r}] = 4^nT_{2n+k,n}.$$

Proof. From Proposition 4.3.11, we can write the left hand side as

$$\begin{aligned}
&\sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)[(ba)^{n-r}\sqcup\!\sqcup(ba)^{n+k+r}]\\
=&\sum_{r=0}^{n}(-1)^r\sum_{j=0}^{n-r}4^j\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\binom{2n+k-2j}{n-r-j}T_{2n+k,j}\\
=&\sum_{j=0}^{n}4^jT_{2n+k,j}\sum_{r=0}^{n-j}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\binom{2n+k-2j}{n-r-j}.
\end{aligned}$$

Thus, it is sufficient to show that the inner sum is 0 for $j \neq n$, and 1 if $j = n$. But this is precisely the statement of Lemma 4.3.12. Hence the result follows. □

As a corollary, we obtain the following identity.

Theorem 4.3.14.

$$\zeta(\{2\}^k\sqcup\!\sqcup\{1,3\}^n)=\frac{\pi^{4n+2k}}{(2n+1)(4n+2k+1)!}\binom{2n+k}{k}.$$

Proof. Evaluating the zeta function on the identity given in Corollary 4.3.13, we obtain

$$\begin{aligned}
\zeta(\{2\}^k\sqcup\!\sqcup\{1,3\}^n)&=4^{-n}\sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\zeta(\{2\}^{n-r})\zeta(\{2\}^{n+k+r})\\
&=4^{-n}\sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\frac{\pi^{4n+2k}}{(2n-2r+1)!(2n+2k+2r+1)!}
\end{aligned}$$

using the well known identity $\zeta(\{2\}^N)=\frac{\pi^{2N}}{(2N+1)!}$. The result then follows from Lemma 4.3.15 □

Lemma 4.3.15.

$$\begin{aligned}
&\frac{4^n}{(2n+1)(4n+2k+1)!}\binom{2n+k}{k}\\
=&\sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\frac{1}{(2n-2r+1)!(2n+2k+2r+1)!}
\end{aligned}$$

for all non-negative n, k.

Proof. Multiplying both sides by $(4n+2k+2)!$, we will prove the equivalent identity

$$2^{2n+1}\binom{2n+k+1}{k} = \sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\binom{4n+2k+2}{2n-2r+1}.$$

Denoting by $[z^N]f(z)$ the coefficient of z^N in a formal power series $f(z)$, we find that the right hand side is given by

$$\begin{aligned}
&[z^{2n-2r-1}]\sum_{r\geq 0}(-1^r)\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)(1+z)^{4n+2k+2}\\
&\quad= [z^{2n+1}](1+z)^{4n+2k+2}\sum_{r\geq 0}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)z^{2r}\\
&\quad= [z^{2n+1}]\frac{(1-z^2)(1+z)^{4n+2k+2}}{(1+z^2)^{k+1}}\\
&\quad= [z^{2n+1}]\frac{(1-z^2)(1+z^2+2z)^{2n+k+1}}{(1+z^2)^{k+1}}\\
&\quad= [z^{2n+1}]\sum_{i=0}^{2n+k+1}\binom{2n+k+1}{i}(1+z^2)^{2n-i}(2z)^i-\binom{2n+k+1}{i}(1+z^2)^{2n-i}2^iz^{i+2}\\
&\quad= [z^0]\sum_{i=0}^{2n+k+1}\binom{2n+k+1}{i}(1+z^2)^{2n-i}2^iz^{i-2n-1}-\binom{2n+k+1}{i}(1+z^2)^{2n-i}2^iz^{i+1-2n}.
\end{aligned}$$

Considering the constant term of this expression, we obtain

$$\sum_{i=0}^{2n}\binom{2n+k+1}{i}\binom{2n-i}{n-\frac{i-1}{2}}2^i-\sum_{i=0}^{2n+1}\binom{2n+k+1}{i}\binom{2n-i}{n-\frac{i+1}{2}}2^i+2^{2n+1}\binom{2n+k+1}{2n+1}$$

where $\binom{N}{K+\frac{1}{2}} := 0$. Clearly, every term with i even vanishes, so this simplifies to the following.

$$\sum_{i=0}^{n}\binom{2n+k+1}{2i+1}\binom{2n-2i-1}{n-i}2^{2i+1}-\sum_{i=0}^{n}\binom{2n+k+1}{2n+1}\binom{2n-2i-1}{n-i-1}2^{2i+1}+2^{2n+1}\binom{2n+k+1}{k}.$$

As $\binom{2n-2i-1}{n-i}=\binom{2n-2i-1}{n-i-1}$, the two sums cancel, and thus we have

$$2^{2n+1}\binom{2n+k+1}{k} = \sum_{r=0}^{n}(-1)^r\left(\binom{k+r}{k}+\binom{k+r-1}{k}\right)\binom{4n+2k+2}{2n-2r+1}.$$

□

Part II

Further Observations

Chapter 5

Finite characteristic, p-adic, and integer solutions to the double shuffle equations

5.1 Shuffle algebras over finite fields

In the 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 [23], 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 non-empty 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 [1].

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 5.1.1. Given an alphabet $X = \{x_1, x_2, \dots, x_n\}$, we define the shuffle algebra $\mathrm{Sh}(R)$ 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

$$u ⧢ 1 = 1 ⧢ u = u,$$

$$x_i u ⧢ x_j v = x_i(u ⧢ x_j v) + x_j(x_i u ⧢ v).$$

It is easy to check that this defines a commutative associative algebra structure on $R\langle X\rangle$.

In particular, if we consider k of positive characterististic p, we find the following decomposition.

Proposition 5.1.2. *Let $\phi_p : Sh(k) \to Sh(k)$ denote the 'shuffle Frobenius' map, sending $u \mapsto u^{⧢ p}$, the shuffle product of p copies of u. Then $Sh(k) = k \oplus ker\phi_p$.*

Proof. First note that, for any commutative product $\boxtimes$, and any $a, b \in \mathbb{F}_p\langle X\rangle$, $(a+b)^{\boxtimes p} = a^{\boxtimes p} + b^{\boxtimes p}$. Hence, ϕ_p is linear, and so, as $\phi_p|_k$ is injective, it suffices to show that for a word u in X, $\phi_p(u) = 0$.

Let $u = x_i v$. Then

$$\begin{aligned}\phi_p(u) &= x_i v ⧢ x_i v ⧢ \cdots x_i v \\ &= \sum_{k=1}^{p} x_i(x_i v ⧢ \cdots ⧢ v ⧢ \cdots ⧢ x_i v),\end{aligned}$$

where we take the x_i from the k^{th} copy of $x_i v$. But as the shuffle product is commutative, we find

$$\begin{aligned}\phi_p(u) &= \sum_{k=1}^{p} x_i(v ⧢ x_i v ⧢ \cdots ⧢ x_i v) \\ &= p x_i(v ⧢ x_i v ⧢ \cdots ⧢ x_i v) = 0.\end{aligned}$$

□

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 $\mathbb{F}_p\langle\langle e_0, e_1\rangle\rangle$ deduce the following result.

Theorem 5.1.3. *There are no non-trivial grouplike elements of $k\langle\langle e_0, e_1\rangle\rangle$ for k a field of positive characteristic p.*

Proof. Suppose $\Phi \in k\langle\langle e_0, e_1\rangle\rangle$ is grouplike. Then we can consider Φ as a homomorphism $\mathrm{Sh}(k) \to k$, mapping a word u to the coefficient of u in $\Phi = \sum_{w\in\{e_0,e_1\}^\times} c_w w$.

As Φ is a homomorphism, we have, for all $w \neq 1$

$$\Phi(w)^p = \Phi(w^{ш p}) = \Phi(0) = 0$$

where the final two equalities follow from Proposition 5.1.2. As the Frobenius map is injective on k, this implies $\Phi(w) = 0$ for all $w \neq 1$, and so $\Phi = \sum_{w\in\{e_0,e_1\}^\times} \Phi(w)w = 1$. □

Corollary 5.1.4. *There exist no non-trivial grouplike elements of $\mathbb{Z}\langle\langle e_0, e_1\rangle\rangle$.*

Proof. Suppose $\Phi = \sum_{w\in\{e_0,e_1\}^\times} c_w w \in \mathbb{Z}\langle e_0, e_1\rangle$ is grouplike. Fix a word $u \neq 1$ in $\{e_0, e_1\}$, and define $u_R^* : R\langle\langle e_0, e_1\rangle\rangle \to R$ to be the R-linear map sending u to 1 and all other words to 0.

Then we have the following commutative diagram and, as a consequence of Theorem

$$\begin{tikzcd}
\mathbb{Z}\langle\langle e_0, e_1\rangle\rangle \arrow[r, "u_{\mathbb{Z}}^*"] \arrow[d] & \mathbb{Z} \arrow[d] \\
\mathbb{F}_p\langle\langle e_0, e_1\rangle\rangle \arrow[r, "u_{\mathbb{F}_p}^*"] & \mathbb{F}_p
\end{tikzcd}$$

(5.1.3), $u_{\mathbb{F}_p}^*$ is the zero map, for all p. Hence, the composition is the zero map. The second

$$\begin{tikzcd}
\mathbb{Z}\langle\langle e_0, e_1\rangle\rangle \arrow[r, "u_{\mathbb{Z}}^*"] & \mathbb{Z} \arrow[r] & \prod_{p \text{ prime}} \mathbb{F}_p
\end{tikzcd}$$

map is injective, and so $u_{\mathbb{Z}}^*$ is the zero map for every $u \neq 1$. Thus $\Phi = 1$. □

Thus we can have no integer grouplike elements of $\mathbb{Q}\langle\langle e_0, e_1\rangle\rangle$.

Remark 5.1.5. The proof of Corollary 5.1.4 is distinctly overkill. The result also follows if we let c_w be the coefficient of some primitive w in Φ, and note that $c_{w^{ш n}} = \frac{c_w^n}{n!}$ for grouplike Φ. As this tends to 0 as n grows, we cannot have every coefficient be integral.

Remark 5.1.6. As noted previously, Theorem 5.1.3 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 $\mathcal{O}_k\langle\langle e_0, e_1\rangle\rangle$.

5.2 The p-adic valuation of coefficients

We can extend Remark 5.1.5 to show grouplike elements of $\mathbb{Z}_p\langle\langle e_0, e_1\rangle\rangle$ cannot exist.

Theorem 5.2.1. *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 can therefore conclude that it is the exponential of a primitive element $\sigma \in \mathbb{Q}_p\langle\langle e_0, e_1\rangle\rangle$.

$$\Phi = \sum_{n\geq 0} \frac{\sigma^n}{n!}.$$

Define a monomial order on $\mathbb{Q}_p\langle e_0, e_1\rangle$ by graded lexicographic ordering, and let w be the minimal word with non-zero coefficient c_w in σ. Note that this will also be a word of minimal weight m. As such, in weight mn, w^n will the the minimal word with respect to the monomial order. We can therefore conclude that the coefficient of w^n will be $\frac{c_w^n}{n!}$, with p-adic valuation

$$n\nu_p(c_w) - \nu_p(n!).$$

As n tends to infinity, this tends to negative infinity. Hence, we cannot have $\Phi \in \mathbb{Z}_p\langle\langle e_0, e_1\rangle\rangle$. □

This provides an immediate answer to a Question 2.26 suggested by Furusho [23] 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 5.2.2. This result is reminiscent of Deligne's description of the motivic fundamental group of a smooth scheme [16]. In describing the ℓ-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 suggests $n = p$ may be sufficient to derive a contradiction.

Corollary 5.2.3. *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* Φ*,* $\nu_p(\Phi) = -\infty$*.*

Proof. Let Φ 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 Φ is trivial by Theorem 5.2.1. Otherwise, if $\nu_p(\Phi) = -N$, for some $N > 0$, consider the element $\widetilde{\Phi} \in \mathbb{Z}_p\langle\langle e_0, e_1\rangle\rangle$ obtained as the image of Φ 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 group like element with finite valuation is trivial. □

Remark 5.2.4. By considering a decomposition $\Phi = 1 + \sum_{n\geq 0} p^n \Phi_n$ into p-adically graded pieces, one can show 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 5.2.5. *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 5.2.4, the p-adic valuation is superadditive with respect to concatenation. Thus, for any factorisation $v = v_1 \dots v_k$, we have $\nu_p(c_v) \geq \nu_p(c_{v_1}) + \cdots + \nu_p(c_{v_k})$. The result follows immediately □

We contrast this result with those of Alekseev, Podkopaeva and Severa [1], who show the following

Theorem 5.2.6. *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 the following as a corollary.

Corollary 5.2.7. *For $p > 2$ prime, let $(\lambda, f) \in GT(\mathbb{Q}_p)$ be such that λ generates a dense subgroup of $\mathbb{Z}_p^*$. Then there exists a unique associator Φ with p-adic coefficients such that*

$$f(\Phi(e_0, e_1)e_0\Phi(e_1, e_0), e_1)\Phi(e_0, e_1) = \Phi(\lambda e_0, \lambda e_1)$$

and satisfying

$$\Phi \in \sum_{n=0}^{\infty} p^{-a_p(n)}\mathbb{Z}_p\langle e_0, e_1\rangle^n,$$

where

$$a_p(n) = \lfloor\frac{n}{p-1}\rfloor + \nu_p\left(\lfloor\frac{n}{p-1}\rfloor!\right).$$

Then, letting $(\lambda', f') := (\lambda, f)^{p-1}$, we have.

$$f' \in 1 + p\mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{\geq 1} + \mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{\geq p-1},$$

and $\psi := ln(f')/ln(\lambda') \in \mathfrak{gt}(\mathbb{Q}_p)$ is of the form

$$\psi \in \mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle + \sum_{s\geq 0} p^{-s-1}\mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{\geq p^s(p-1)}$$

where GT and $\mathfrak{gt}$ are the (prounipotent) Grothendieck-Teichmuller group and Lie algebra, respectively, $\mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle^{\geq n}$ denotes the set of elements of $\mathbb{Z}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle$ of degree at least n, and $\hat{e}_i := exp(e_i) - 1$.

While this gives quite a strong bound on the growth of coefficients of elements of $GT(\mathbb{Q}_p)$, we cannot immediately apply this to rational associators, as not all elements of $\mathbb{Q}$ generate a dense subgroup of $\mathbb{Z}_p^*$. Additionally, the strength of this bound, giving at most logarithmic growth of the valuation, is true for $\psi \in \mathbb{Q}_p\langle\langle\hat{e}_0, \hat{e}_1\rangle\rangle$. Translating this back to $\psi \in \mathbb{Q}_p\langle\langle e_0, e_1\rangle\rangle$ gives at most linear growth of the valuation, in line with results of Corollary 5.2.5.

Chapter 6

Defining orthogonal generators and observations on duality

6.1 Canonical elements

As mentioned in Part 1, one of the strengths of the block graded approach is that $\mathfrak{bg}$ has generators with canonical presentations. Reproducing this canonical presentation for generators of $\mathfrak{g}^{\mathfrak{m}}$, in order to have an explicit generating set, would be a great step forward in describing motivic relations. There seem to be four possible approaches to providing such an explicit set : using inner products and a Gram-Schmidt-like procedure, using a basis of multiple zeta values, Brown's anatomical decomposition, or finding a section of the block projection. The first approach has not been seen in the literature to this point, and so we focus on this, finding several new results.

Theorem 6.1.1 (Keilthy, Hain)**.** *Given a choice of inner product on* $\mathbb{Q}\langle e_0, e_1\rangle$ *and normalisation of* $(\sigma_{2k+1}, e_1 e_0^{2k})$*, we can define a unique embedding of* $\{\sigma_3, \sigma_5, \sigma_7, \ldots\} \hookrightarrow \mathbb{Q}\langle e_0, e_1\rangle$*, and hence of the motivic Lie algebra.*

Proof. Suppose that we have a fixed embedding of $\sigma_3, \ldots, \sigma_{2k-1}$ into $\mathbb{Q}\langle e_0, e_1\rangle$ and consider the space $\mathrm{Lie}(\sigma_3, \ldots, \sigma_{2k+1})_{2k+1}$, where the subscript denotes the sub-vector space spanned by elements of weight $2k+1$. This contains $\mathrm{Lie}(\sigma_3 \ldots, \sigma_{2k-1})_{2k+1}$ as a codimension 1 subspace, and, as it is finite dimensional, the inner product restricts to a non-degenerate inner product. Hence, we can fix σ_{2k+1} up to a scalar multiple by imposing orthogonality of σ_{2k+1} to $\mathrm{Lie}(\sigma_3, \ldots, \sigma_{2k-1})_{2k+1}$. Thus, as σ_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 σ_{2k+1} up to rescaling. A fixed choice of normalisation then completely determines the embedding. □

There a natural candidate for our inner product $\langle \cdot, \cdot \rangle : \mathbb{Q}\langle a, b\rangle \times \mathbb{Q}\langle a, b\rangle \to \mathbb{Q}$. Define, for monic monomials u and v,

$$\langle u, v\rangle_{triv} := \begin{cases} 1 & \text{if } u = v \\ 0, & \text{otherwise} \end{cases}$$

and extend by linearity. It is easy to check that this satisfies the requirements of an inner product.

Example 6.1.2. By considering the trivial inner product of the depth 3 components of σ_{11} and $\{\sigma_3, \{\sigma_3, \sigma_5\}\}$, and demanding that these be orthogonal, we find the following canonical decomposition of σ_{11}:

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

where we have omitted terms of depth 5 (that are uniquely determined), and where ψ_{2n+1} is given by Definition 10.1 of [12].

Remark 6.1.3. 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 involves grow quite rapidly.

This has the advantage of being easy to calculate, with monomials of different weights and depths being orthogonal, but is not "compatible" with the obvious Lie algebra structure on $\mathbb{Q}\langle a, b\rangle$, nor with the Ihara bracket. Indeed, it would be particularly interesting to find such an inner product. Evidence coming from the work of Pollack [37] suggests the existence of one, but gives no hints as to how to construct it.

One should note that, while the trivial inner product seems rather artificial, it actually has Hodge theoretic origins. Due to the inclusion

$$\mathbb{P}^1 \setminus \{0,1,\infty\} \hookrightarrow E^{\times}_{\frac{\partial}{\partial q}}$$

into the first order Tate curve, we obtain an inclusion

$$\mathfrak{g}^{\mathfrak{m}} \to \mathrm{Lie}\pi_1^{un}(E^{\times}_{\frac{\partial}{\partial q}})^{dR}.$$

Hodge theoretic arguments give a splitting $H_1^{dR}(E^{\times}_{\frac{\partial}{\partial q}}) = \mathbb{Q}A \oplus \mathbb{Q}T$ [28], with a natural inner product satisfying $\langle A, T\rangle = 0$, corresponding to the trivial inner product.

Other authors have suggested candidates for canonical generators. For example, in [13], Brown defines a family of $\{\sigma^c_{2n+1}\}$ in terms of Bernoulli numbers. These solve the double shuffle equations modulo products up to depth three and give interesting ties to $\mathfrak{sl}_2$ and period polynomials, that also arise in the work of Pollack [37]. Specifically, the coefficients appearing in these σ^c_{2n+1} are proportional to those of the odd part of the period polynomial for the Eisenstein series of weight $2n$, which is proportional to:

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

We have checked that this “anatomical” decomposition, and the trivial inner product give distinct generators, but it would be interesting to see if there existed a reasonable inner product giving Brown’s proposed generators.

6.2 The duality phenomenon

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

Definition 6.2.1. Define the following linear maps on $\mathbb{Q}\langle a, b\rangle$.

- $R(u_1u_2\dots u_n) := u_nu_{n-1}\dots u_1$,
- W is the homomorphism defined by $Wa := b$ and $Wb := a$,
- $\mathrm{D} := RW = WR$.

We say σ satisfies *duality* if $\sigma = \mathrm{D}\sigma$.

We have $\zeta(w) = \zeta(\mathrm{D}w)$, 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 $\sigma = \mathrm{D}\sigma$ for all $\sigma \in \mathfrak{dmr}_0$. 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 6.2.2. The map R defined here is, up to a sign, the antipode map S in the shuffle Hopf algebra $\mathbb{Q}\langle a, b\rangle$. Specifically, if w is a word of length n, then $Rw = (-1)^n Sw$.

However, we do know that duality plays nicely with many of the structures on $\mathfrak{g}^{\mathfrak{m}}$ and $\mathfrak{dmr}_0$: D passes through the motivic coaction [9] and duality is preserved by the Ihara bracket. While this latter fact follows from Brown's proof that the Ihara action is motivic [10], and Racinet's thesis [38], we will present a direct proof of it.

Lemma 6.2.3 (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. In a Hopf algebra with coproduct Δ and antipode S, it is a standard result that if ϕ is primitive with respect to Δ, then $\phi + S\phi = 0$. If $\phi(a, b)$ satisfies the shuffle equations mod products, then it is primitive and hence

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

Applying D to this proves our result. ☐

Theorem 6.2.4 (K.)**.** *Duality is preserved in $\mathfrak{dmr}_0$ by the Ihara bracket.*

Proof. Recall that 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_ϕ is the derivation defined on generators by

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

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

Now suppose $\phi_1, \phi_2 \in \mathfrak{dmr}_0$ 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'_ϕ by

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

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

We can easily show by induction on the length of ϕ 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 $\mathrm{D}\{\phi_1, \phi_2\} = -\{\phi_1, \phi_2\}(-b, -a) = \{\phi_1, \phi_2\}$. $\square$

As such, it would suffice to show $D\phi = \phi$ for a generating set. We first note that D preserves solutions to the shuffle equations.

Lemma 6.2.5 (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

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

Thus

$$(\mathrm{D} \otimes \mathrm{D}) \circ \Delta = \Delta \circ \mathrm{D}$$

proving our result. $\square$

We can now show the following result. While it is not known that $\{\sigma_{2k+1}\}_{k\geq 1}$ generate $\mathfrak{dmr}_0$, and duality is known to hold for all of $\mathfrak{g}^{\mathfrak{m}}$ for motivic reasons, it is still interesting to see that it can be derived from the double shuffle equations with some minor assumptions, and suggests a possible route for further exploration.

Proposition 6.2.6 (K.). *Suppose* $\sigma_3, \ldots, \sigma_{2k-1}$ *satisfy duality. Suppose also that* $D\sigma_{2k+1} \in \mathfrak{g}^{\mathfrak{m}}$. *Then* σ_{2k+1} *satisfies duality.*

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

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

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

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

and so

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

Now, if $\alpha = -1$, then

$$(\sigma_{2k+1} - \alpha\mathrm{D}\sigma_{2k+1}|a^{2k}b) = 2(\sigma_{2k+1}|a^{2k}b) \neq 0.$$

But any sum of brackets of lower weight cannot have any terms of depth one, so we must have

$$(\sigma_{2k+1} - \alpha\mathrm{D}\sigma_{2k+1}|a^{2k}b) = 0.$$

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

One could alter the assumptions made about $\mathrm{D}\sigma_{2k+1}$, however, it is not clear that the altered assumptions would be weaker. For example, if we simply take $\mathrm{D}\sigma_{2k+1} \in \mathfrak{dmr}_0$ [40] 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 σ_{2k+1} by an arbitrary element, as we rely on having non-zero depth one components, and in this, σ-elements are near unique in $\mathfrak{dmr}_0$.

Part III

References

Chapter 7

Glossary of symbols

As we introduce many notions in this thesis, we include a short summary of some of the important notations.

$\mathcal{H}$: The $\mathbb{Q}$-algebra of motivic multiple zeta values.

$\mathrm{I}^{\mathfrak{m}}(\bullet)$: The motivic iterated integral associated to to $\bullet$. Here, $\bullet$ could be a word in $\{0,1\}$, $\{e_0,e_1\}$, $\{y_1,y_2,\ldots\}$ or $\{z_1,z_2,\ldots\}$. The image under the period map of $\mathrm{I}^{\mathfrak{m}}(\bullet)$ is the associated shuffle-regularised iterated integral.

$\zeta^{\mathfrak{m}}(\bullet)$: A motivic multiple zeta value. This differs from $\mathrm{I}^{\mathfrak{m}}(\bullet)$ by a factor of $(-1)^d$, where d is the depth of $\bullet$.

$\mathcal{A}$: The $\mathbb{Q}$-algebra of de Rham multiple zeta values, $\mathcal{A}\cong\mathcal{H}/(\zeta^{\mathfrak{m}}(2))$. This can be considered as the space of multiple zeta values modulo $\zeta(2)$.

$\mathrm{I}^{\mathfrak{a}}(\bullet)$: The de Rham iterated integral associated to $\bullet$.

$\zeta^{\mathfrak{a}}(\bullet)$: The de Rham multiple zeta value associated to $\bullet$. This differs from $\mathrm{I}^{\mathfrak{a}}(\bullet)$ by a factor of $(-1)^d$, where d is the depth of $\bullet$.

$\mathcal{L}$: The Lie coalgebra of motivic multiple zeta values, $\mathcal{L}=\frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0}\mathcal{A}_{>0}}$, where $\mathcal{A}_{>0}=\mathcal{A}\setminus\mathbb{Q}$. This can be considered as the space of multiple zeta values modulo products.

$\mathrm{I}^{\mathfrak{l}}(\bullet)$: The image of $\mathrm{I}^{\mathfrak{a}}(\bullet)$ in $\mathcal{L}$.

$\mathfrak{g}^{\mathfrak{m}}$: The motivic Lie algebra. This is the Lie algebra of the unipotent part of the motivic Galois group $G_{\mathcal{MT}(\mathbb{Z})}$, and the dual of $\mathcal{L}$. It is non-canonically isomorphic to to the free Lie algebra on $\{\sigma_{2k+1}\}_{k\geq 1}$, and can be embedded into $\mathbb{Q}\langle e_0, e_1\rangle$. It encodes relations among elements of $\mathcal{L}$.

$\mathcal{W}$: The weight filtration. An increasing filtration on $\mathcal{H}$, such that $\mathrm{I}^{\mathfrak{m}}(0; w; 1) \in \mathcal{W}_n\mathcal{H}$ if $|w| \leq n$. This is a grading on $\mathcal{H}$, and conjecturally remains a grading upon taking the period map. $\mathcal{W}$ is also used to refer to the induced filtrations on $\mathcal{A}$ and $\mathcal{L}$, along with the dual decreasing filtration on $\mathfrak{g}^{\mathfrak{m}}$.

$\mathcal{D}$: The depth filtration. An increasing filtration on $\mathcal{H}$ such that $\mathrm{I}^{\mathfrak{m}}(0; w; 1) \in \mathcal{D}_n\mathcal{H}$ if 1 appears at most n times in w. This is not a grading on $\mathcal{H}$, but is an algebra filtration for both shuffle and stuffle products. Like $\mathcal{W}$, $\mathcal{D}$ is used to refer to all induced filtrations.

$\mathfrak{dg}$: The associated graded Lie algebra of $\mathfrak{g}^{\mathfrak{m}}$ with respect to the depth filtration: $\mathfrak{dg} = \bigoplus_{n=1}^{\infty} \mathcal{D}^n\mathfrak{g}^{\mathfrak{m}}/\mathcal{D}^{n+1}\mathfrak{g}^{\mathfrak{m}}$. This describes relations among depth graded motivic multiple zeta values. It is not a free Lie algebra, with quadratic relations arising from a connection to period polynomials of modular forms.

We also defined the following notions.

$\mathrm{I}^{\mathfrak{f}}(\bullet)$: The formal iterated integral associated to $\bullet$. The formal iterated integrals are purely formal symbols and satisfy no relations. The motivic coaction, applied purely symbolically to the span of such formal symbols $\mathcal{I}$ defines a coproduct. We have a natural surjective map from $\mathcal{I}$ to both $\mathcal{H}$ and $\mathcal{A}$ that commutes with the computation of the coaction.

$\mathcal{B}$: The block filtration. An increasing filtration on $\mathcal{H}$ such that $\mathrm{I}^{\mathfrak{m}}(0; w; 1) \in \mathcal{B}_n\mathcal{H}$ if $0w1$ can be decomposed into at most $n+1$ alternating blocks of maximal length. Equivalently if $0w1$ contains at most n occurrences of the subsequences 00 or 11. It is also used to refer to all induced filtrations. The block filtration agrees with the coradical filtration associated to the motivic coaction.

$\deg_{\mathcal{B}}(\bullet)$: The block degree of the word $\bullet$. If $\bullet$ is a word in $\{e_0, e_1\}$, then $\deg_{\mathcal{B}}(\bullet)$ is the number of occurrences of the subwords e_0e_0 or e_1e_1.

$\mathrm{I}^{\mathfrak{b}}(\bullet)$: The block graded motivic iterated integral associated to $\bullet$. If $\deg_{\mathcal{B}}(\bullet) = n$, this denotes the image of $\mathrm{I}^{\mathfrak{m}}(\bullet)$ in $\mathcal{B}_n\mathcal{H}/\mathcal{B}_{n-1}\mathcal{H}$.

$\zeta^{\mathfrak{b}}(\bullet)$: The block graded motivic multiple zeta value associated to $\bullet$. This differs from $\mathrm{I}^{\mathfrak{b}}(\bullet)$ by a factor of $(-1)^d$, where d is the depth of $\bullet$.

$\mathrm{I}^{\mathfrak{bl}}(\bullet)$: This is the image of $\mathrm{I}^{\mathfrak{b}}(\bullet)$ in $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$. These span the space of motivic multiple zeta values modulo products and terms of lower block degree.

$\zeta^{\mathfrak{bl}}(\bullet)$: The block graded motivic multiple zeta value modulo products associated to $\bullet$. This differs from $\mathrm{I}^{\mathfrak{bl}}(\bullet)$ by a factor of $(-1)^d$, where d is the depth of $\bullet$.

$\mathfrak{bg}$: The block graded motivic Lie algebra: $\mathfrak{bg} = \bigoplus_{n=1}^{\infty} \mathcal{B}^n\mathfrak{g}^{\mathfrak{m}}/\mathcal{B}^{n+1}\mathfrak{g}^{\mathfrak{m}}$. This is a free Lie algebra and $\mathfrak{bg} \cong \mathfrak{g}^{\mathfrak{m}}$. It is dual to $\mathrm{gr}^{\mathcal{B}}\mathcal{L}$, and so describes relations among motivic multiple zeta values modulo products and terms of lower block degree.

$\mathfrak{rbg}$: The reduced block graded Lie algebra : The image of $\mathfrak{bg} \hookrightarrow \bigoplus_{n=2}^{\infty} \mathbb{Q}[x_1, \ldots, x_n]$ lies in the vector subspace $\bigoplus_{n=2}^{\infty} x_1 \ldots x_n(x_1 - x_n)\mathbb{Q}[x_1, \ldots, x_n]$. We have an injection

$$x_1 \ldots x_n(x_1 - x_n)\mathbb{Q}[x_1, \ldots, x_n] \hookrightarrow \mathbb{Q}[x_1, \ldots, x_n]$$

given by division by $x_1 \ldots x_n(x_1 - x_n)$. $\mathfrak{rbg}$ is the image of $\mathfrak{bg}$ under the composition of these two injections. $\mathfrak{rbg} \cong \mathfrak{bg}$, but we find additional symmetries in this presentation.

Chapter 8

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