On the Broadhurst-Kreimer generating series for multiple zeta values

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Abstract. Let $\mathcal{F}$ denote the free polynomial algebra $\mathcal{F} = \mathbb{Q}\langle s_3, s_5, s_7, \ldots\rangle$ on non-commutative variables s_i for odd $i \geq 3$. The algebra $\mathcal{F}$ is weight-graded by letting s_n be of weight n; we write $\mathcal{F}_n$ for the weight n part. In this paper we put a "special" decreasing depth filtration

$$\mathcal{F} = \mathcal{F}^1 \supset \mathcal{F}^2 \supset \cdots \supset \mathcal{F}^d \supset \mathcal{F}^{d+1} \cdots$$

on $\mathcal{F}$, based on the period polynomials associated to cusp forms on $\mathrm{SL}_2(\mathbb{Z})$. We define a lattice L of particular combinatorially defined subspaces of $\mathcal{F}$, and conjecture that this lattice is distributive. Assuming this conjecture, we show that the dimensions of the weight n filtered quotients $\mathcal{F}_n^d/\mathcal{F}_n^{d+1}$ are given by the coefficients of the well-known Broadhurst-Kreimer generating series, defined by them to predict dimensions for the algebra of multiple zeta values. We end by explaining the expected relationship between $\mathcal{F}$ equipped with the special depth filtration and the algebras of formal and motivic multiple zeta values.

1. Introduction

Let $\mathcal{F} = \mathbb{Q}\langle s_3, s_5, s_7, \ldots\rangle$ be the free polynomial algebra generated by elements s_i, $i \geq 3$ odd. The algebra $\mathcal{F}$ is equipped with a weight grading $\mathcal{F} = \oplus_{n\geq 3}\mathcal{F}_n$ given by associating the weight i with each s_i and extending the weight additively to products. Also, $\mathcal{F}$ is equipped with a standard depth grading for which a monomial is of depth d if it is a product $s_{i_1}\cdots s_{i_d}$. In this text we will equip $\mathcal{F}$ with another structure, called the *special depth filtration*, which is a decreasing filtration $\mathcal{F}^1 \supset \mathcal{F}^2 \supset \cdots$ on $\mathcal{F}$, which thus induces a filtration $\mathcal{F}_n^1 \supset \mathcal{F}_n^2 \supset \cdots$ also on each graded part of $\mathcal{F}$.

The main goal of this paper is to compare the dimensions of the associated graded of $\mathcal{F}$ for the special depth filtration with the coefficients of the famous Broadhurst-Kreimer generating series for multiple zeta values. Broadhurst and Kreimer defined the following 2-variable rational function:

$$BK(X,Y) = \frac{1}{1 - O(X)Y + S(X)Y^2 - S(X)Y^4}, \tag{1.1}$$

where

$$O = O(X) = \frac{X^3}{1-X^2} = \sum_{i=1}^{\infty} X^{2i+1}$$

and

$$S = S(X) = \frac{X^{12}}{(1-X^4)(1-X^6)} = \sum_{\substack{n=12 \\ n \text{ even}}}^{\infty} sp(n) X^n,$$

where $sp(n) = \lfloor \frac{n-4}{4} \rfloor - \lfloor \frac{n-2}{6} \rfloor$ is the dimension of the space $S_n(\mathrm{SL}_2(\mathbb{Z}))$ of weight n cusp forms on the full modular group. Their conjecture states that the coefficient of $X^n Y^d$ in the Taylor expansion of this function around $(0,0)$ is equal to the number of linearly independent multiple zeta values of weight n and depth d (see §7). In this paper, we state a conjecture on a certain lattice of combinatorially defined subspaces of the free algebra $\mathcal{F}$, and then, assuming this conjecture, prove that the coefficients of the Broadhurst-Kreimer series do actually give the dimensions of the graded pieces of the associated graded of $\mathcal{F}$ with respect to the special depth filtration.

In §2, we recall the definition of the period polynomials associated to cusp forms on $\mathrm{SL}_2(\mathbb{Z})$, and use them to define the special depth filtration on the free algebra $\mathcal{F}$. In §3 we give a preliminary version of the distributivity conjecture and state our main results on the Broadhurst-Kreimer generating series and the dimensions of the associated graded pieces of $\mathcal{F}$ for the special depth filtration. In §4 we define the lattice of subspaces we need to consider in $\mathcal{F}$, and give the precise statement of our main conjecture. Sections §§5-6 are devoted to the proofs. Finally, in §7, we discuss the relation of this theorem to formal and motivic multiple zeta values.

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2. Period polynomials and the special depth filtration

Definition 2.1. A polynomial $P(X) \in \mathbb{Q}[X]$ is said to be a *period polynomial of weight n with respect to* $\mathrm{SL}_2(\mathbb{Z})$ if it is a polynomial of degree $\leq n-2$ satisfying the following two equalities:

$$P(X) + X^{n-2} P(\frac{-1}{X}) = 0,$$

$$P(X) + X^{n-2} P(1 - \frac{1}{X}) + (X-1)^{n-2} P(\frac{1}{1-X}) = 0.$$

We say that $P(X)$ is an *even* period polynomial if $P(X) = P(-X)$, and a *reduced even* period polynomial if $P(X)$ is even, $\deg P \leq n-4$, and $P(0) = 0$. The reduced even period polynomials of weight n form a vector space over $\mathbb{Q}$ which we denote by $\mathcal{P}_n$.

Remark 2.2. Consider the integral

$$r_f(X) = \int_0^{i\infty} f(z)(z-X)^{n-2} dz$$

attached to a weight n modular form f on $\mathrm{SL}_2(\mathbb{Z})$. Set

$$r_f^+(X) = \frac{1}{2}\big(r_f(X) + r_f(-X)\big);$$

then $r_f^+(X)$ is an even polynomial. Let $R_f^+(X)$ denote the *reduced* even period polynomial obtained from the even period polynomial $r_f^+(X)$ by removing the term of degree $n-2$ and the constant term (if any). Up to scalar multiple, the even period polynomial associated to the weight n Eisenstein series G_n is $X^{n-2}-1$, so that in fact the reduced even period polynomial $R_f^+(X)$ is always the even period polynomial $r_g^+(X)$ of a unique linear combination g of f and G_n. The Eichler-Shimura correspondence shows that $f \mapsto r_f^+(X)$ yields an isomorphism between the vector space $M_n\big(\mathrm{SL}_2(\mathbb{Z})\big)$ of modular forms of weight n on $\mathrm{SL}_2(\mathbb{Z})$ and the vector space of even period polynomials, which then induces an isomorphism $f \mapsto R_f^+(X)$ between the space $S_n\big(\mathrm{SL}_2(\mathbb{Z})\big)$ of cusp forms of weight n on $\mathrm{SL}_2(\mathbb{Z})$ and the space $\mathcal{P}_n$ of reduced even period polynomials. In particular, it follows that

$$\dim \mathcal{P}_n = \dim S_n\big(\mathrm{SL}_2(\mathbb{Z})\big) = sp(n) = \lfloor (n-4)/4 \rfloor - \lfloor (n-2)/6 \rfloor.$$

In particular, the first values of n for which $\dim \mathcal{P}_n \neq 0$ are $n = 12, 16, 18, \ldots$ The identity of the period polynomials (resp. the even, odd, reduced even ones) defined this way and those of Definition 2.1 can be found for example in [**19**].

Example 2.3. In weight 12, there is a degree 8 period polynomial given by

$$P(X) = X^8 - 3X^6 + 3X^4 - X^2 \tag{2.1}$$

which is the reduced period polynomial associated to the Ramanujan Δ cusp form.

Using the period polynomials, we can now give the definition of the special depth filtration on the free algebra $\mathcal{F}$. We first need to define the subspaces of *special elements* of $\mathcal{F}$.

Definition 2.4. Let $\mathcal{S}_n$ be the image of $\mathcal{P}_n$ under the map $\rho_n : \mathcal{P}_n \to \mathcal{F}$ given by

$$P(X) = \sum_i a_i (X^{2i} - X^{n-2-2i}) \mapsto \sum_i a_i \big(s_{2i+1} s_{n-2-2i+1} - s_{n-2-2i+1} s_{2i+1} \big).$$

By definition, $\mathcal{S}_n$ is a vector subspace of the graded weight n part $\mathcal{F}_n$ of $\mathcal{F}$. Since the maps ρ_n are obviously injective, we have $\dim(\mathcal{S}_n) = \mathrm{sp}(n) = \lfloor (n-4)/4 \rfloor - \lfloor (n-2)/6 \rfloor$. For convenience, we write $\mathcal{S}$ for the union of the underlying sets of the spaces $\mathcal{S}_n$, $n \geq 12$. Elements of $\mathcal{S}$ are *special elements* of $\mathcal{F}$.

Let us also introduce a notation for the standard depth filtration: for $j \geq 1$, we write $D^j\mathcal{F}$ for the j-th part of the ordinary depth grading on $\mathcal{F}$, so $D^j\mathcal{F}$ is the vector subspace of $\mathcal{F}$ generated by all monomials $s_{i_1} \cdots s_{i_j}$.

Definition 2.5. The special depth filtration on $\mathcal{F}$ is defined as follows. For $j = 1, 2, 3$, let $V^i\mathcal{F} = D^i\mathcal{F}$. Let $V^4\mathcal{F}$ be the vector subspace generated by $D^4\mathcal{F}$ and also by the elements of all the subspaces $\mathcal{S}_n \subset V^2\mathcal{F} \subset \mathcal{F}$. For $j \geq 5$, let $V^j\mathcal{F}$ be generated by products ST where $S \in V^k\mathcal{F}$ and $T \in V^l\mathcal{F}$ with $k + l = j$, with $k, l \geq 1$.[1] We define the *special depth filtration* on $\mathcal{F}$ by

$$\mathcal{F}^d = \langle \bigcup_{i \geq d} V^i\mathcal{F} \rangle.$$

[1]Note in particular that $\mathcal{S}_n = V^2\mathcal{F}_n \cap V^4\mathcal{F}_n$ for each n, and in general, $V^j\mathcal{F} \cap V^{j+2}\mathcal{F} \neq 0$.

3. Distributivity conjecture and Broadhurst-Kreimer dimensions

In this section, we state our main results on the relation between the coefficients of the expansion around $(0,0)$ of the Broadhurst-Kreimer generating function

$$BK(X,Y) = \sum_{n\geq 0, d\geq 0} c_n^d X^n Y^d \qquad (4.1)$$

and the dimensions of the weight-graded parts of the associated graded of $\mathcal{F}$ for the special depth filtration. Our results depend on conjectural properties of certain subspaces $\mathcal{F}_n^K \subset \mathcal{F}$, the *shuffle subspaces*, whose precise definition can be found in §4. The statement of our conjecture is as follows. Let $\mathcal{L}$ denote the lattice (in the sense of order theory) of subspaces of $\mathcal{F}$ generated by the shuffle subspaces, i.e. $\mathcal{L}$ contains the shuffle subspaces and is closed under intersections and sums.

Conjecture 3.1. *The lattice $\mathcal{L}$ is distributive, i.e. for any $U, V, W \in \mathcal{L}$, we have*

$$U \cap (V + W) = U \cap V + U \cap W.$$

Remark 3.2. This conjecture is equivalent to the statement that the algebra $\mathcal{F}/I(\mathcal{S})$ is Koszul, where $I(\mathcal{S})$ is the ideal of $\mathcal{F}$ generated by $\mathcal{S}$. For a discussion of this and other equivalent formulations related to the Broadhurst-Kreimer conjecture, see [**8**].

Theorem 3.3. *Assume Conjecture 3.1. Then the coefficient c_n^d of the Taylor expansion of $BK(X,Y)$ around $(0,0)$ is equal to the dimension of the quotient of successive filtered pieces of $\mathcal{F}_n$ by the special depth filtration:*

$$c_n^d = \dim \mathcal{F}_n^d / \mathcal{F}_n^{d+1}.$$

In particular, if $n \not\equiv d$ mod 2, then

$$c_n^d = \dim \mathcal{F}_n^d / \mathcal{F}_n^{d+1} = 0,$$

i.e. $\mathcal{F}_n^d = \mathcal{F}_n^{d+1}$ if $n \not\equiv d$ mod 2.

Theorem 3.3 will follow as an easy corollary of the more detailed Theorem 3.4, which makes use of the standard depth grading on $\mathcal{F}$. Let $\mathcal{F}_{n,k}$ denote the subspace of $\mathcal{F}$ generated by monomials of standard depth k (i.e. products of k s_i's) of weight n, so $\mathcal{F}_n = \oplus_{k\geq 1} \mathcal{F}_{n,k}$. In fact, the standard depths that can occur for weight n are limited. In particular, no elements of standard depth k can occur in weight n if $n \not\equiv k$ mod 2. Moreover, we have

$$\mathcal{F}_n = \bigoplus_{k=1}^{\lfloor n/3 \rfloor} \mathcal{F}_{n,k}, \qquad (3.1)$$

as the maximal possible standard depth in weight n occurs when $n \equiv 0$ mod 3 for the monomial $s_3^{n/3}$.

The special depth filtration induces a filtration on each $\mathcal{F}_n$ and on each $\mathcal{F}_{n,k}$.

For the next theorem, we introduce a refined version of the Broadhurst-Kreimer function, with three variables, as follows:

$$\widetilde{BK}(X,Y,Z) = \frac{1}{1 - O(X)YZ + S(X)Y^2Z^2(1-Z^2)}.$$

Clearly $\widetilde{BK}(X,1,Y) = BK(X,Y)$. Furthermore, $\widetilde{BK}(X,Y,1)$ is a generating series for the filtered quotients of $\mathcal{F}$ equipped with the standard filtration.

THEOREM 3.4. (i) *Unless $n \equiv k \equiv d$ mod 2, we have $\mathcal{F}^d_{n,k}/\mathcal{F}^{d+1}_{n,k} = 0$.*

(ii) *Assume Conjecture 3.1, and let $e^d_{n,k}$ be the coefficient of $X^nY^kZ^d$ in the Taylor series of $\widetilde{BK}(X,Y,Z)$. Then*

$$e^d_{n,k} = \dim \mathcal{F}^d_{n,k}/\mathcal{F}^{d+1}_{n,k}. \tag{3.2}$$

PROOF OF THEOREM 3.3, using Theorem 3.4. By (3.1), we have

$$\mathcal{F}^d_n = \bigoplus_{k=1}^{\lfloor n/3\rfloor} \mathcal{F}^d_{n,k}. \tag{3.3}$$

We first observe that if $k > d$, then $\mathcal{F}^d_{n,k} = \mathcal{F}^{d+1}_{n,k}$. Indeed, the special depth of an element is always greater than or equal to its standard depth; in particular the special depth of an element of standard depth k is at least k, so if $k > d$, then the special depth is also greater than d. Thus if $k > d$, any element of $\mathcal{F}^d_{n,k}$ also lies in $\mathcal{F}^{d+1}_{n,k}$, so these spaces are equal.

Thus we find that quotienting $\mathcal{F}^d_n$ by $\mathcal{F}^{d+1}_n$ gives the direct sum of quotients

$$\mathcal{F}^d_n/\mathcal{F}^{d+1}_n = \bigoplus_{k=1}^{\lfloor n/3\rfloor} \mathcal{F}^d_{n,k}/\mathcal{F}^{d+1}_{n,k} = \bigoplus_{k=1}^{d} \mathcal{F}^d_{n,k}/\mathcal{F}^{d+1}_{n,k}. \tag{3.4}$$

using (3.3) for the first equality and the above observation to reduce the upper limit of the sum from $\lfloor n/3\rfloor$ to d. But it follows from (3.2) of Theorem 3.4 that the dimension of the right-hand term of (4.5) is $\sum_{k=1}^d e^d_{n,k}$, and by the equality $\widetilde{BK}(X,1,Y) = BK(X,Y)$, we have

$$\sum_{k=1}^{d} e^d_{n,k} = c^d_n. \tag{3.5}$$

This proves the first statement of Theorem 3.3.

The second statement of Theorem 3.3 follows immediately from Theorem 3.4 (i) by summing over k. □

4. Shuffle subspaces of $\mathcal{F}$

In this section we make the statement of Conjecture 3.1 precise by defining the *shuffle subspaces* of $\mathcal{F}$, and prove some properties that will be necessary for the proof of Theorem 3.4.

We start by considering the subspaces $\mathcal{F}^d_{n,k}$ with $d \equiv k$ mod 2 (indeed, it will be shown in the proof of part (i) of Theorem 3.4 below that these spaces are zero when $d \not\equiv k$ mod 2). The main remark is that $\mathcal{F}^d_{n,k}$ is generated by the set of possible products, in any order, of $a = (d-k)/2$ special elements and $d-4a$ single s_i's, of total weight n. The definition of a ensures that the standard depth of such a product is given by $d-2a = k$, and the special depth is equal to d. We say that such a product is of type $(a, d-4a)$, so these products generate $\mathcal{F}^d_{n,k} = \mathcal{F}^d_{n,d-2a}$. Let us illustrate this with an example.

Note that given a monomial in elements s_i and special elements $S \in \mathcal{S}$, its degree k as a polynomial in the s_i is given by the number of s_i plus twice the number a of special elements S in the monomial. We write $d = 2a + k$; this d measures the special depth of the monomial, i.e. its position in the special depth filtration. Each s_i in the monomial adds 1 to the count of d, and by the definition of the special depth filtration, each S adds 4.

EXAMPLE 4.1. Let $n = 24$. In the case where $d = 6$ and $a = 1$ (so $k = 4$), the space $\mathcal{F}^6_{24,4}$ is generated by "monomials" that are products of two single s_i and one special element in $\mathcal{S}$; the possibilities are

$$s_3s_9S_{12},\ s_5s_7S_{12},\ s_7s_5S_{12},\ s_9s_3S_{12},\ s_3S_{12}s_9,\ s_5S_{12}s_7,\ s_7S_{12}s_5,\ s_9S_{12}s_3,\ S_{12}s_3s_9,$$

$$S_{12}s_5s_7,\ S_{12}s_7s_5, S_{12}s_9s_3,\ s_3s_5S_{16},\ s_5s_3S_{16},\ s_3S_{16}s_5,\ s_5S_{16}s_3,\ S_{16}s_3s_5,\ S_{16}s_5s_3,$$

$$s_3^2S_{18},\ s_3S_{18}s_3,\ S_{18}s_3^2,$$

where $S_{12} = [s_3, s_9] - 3[s_5, s_7]$ generates $\mathcal{S}_{12}$, $S_{16} = 2[s_3, s_{13}] - 7[s_5, s_{11}] + 11[s_7, s_9]$ generates $\mathcal{S}_{16}$, and $S_{18} = 8[s_3, s_{15}] - 25[s_5, s_{13}] + 26[s_7, s_{11}]$ generates $\mathcal{S}_{18}$.

If we now consider the case where $d = 8$ and $a = 2$ (so again $k = 4$), the space $\mathcal{F}^8_{24,4}$ is one-dimensional, generated by the single element S_{12}^2.

This example shows that each of the vector spaces $\mathcal{F}^d_{n,d-2a}$ possesses natural subspaces determined by the order of the terms, more precisely by the positions or slots occupied by the special elements S between the single s_i. Decomposition into these subspaces will be essential in computing Broadhurst-Kreimer dimensions.

Let us introduce a notation to describe the subspace of $\mathcal{F}^d_{n,d-2a}$ spanned by products of a special elements and $d - 4a$ single s_i in which the special elements occur in prescribed places.

DEFINITION 4.2. For each choice of $d, a \geq 0$ with $d \geq 4a$, let $sh(a, d - 4a)$ denote the set of shuffles of a S's and $d - 4a$ s's, giving words of total length $d - 2a$. For example, $sh(2, 3)$ is given by

$$\{SSsss, SsSss, SssSs, SsssS, sSSss, sSsSs, sSssS, ssSSs, ssSsS, sssSS\}$$

is the set of shuffles of two S's and three s's, corresponding to the values $a = 2$, $d = 11$. Another way of viewing these shuffles is as the set of ordered partitions of a sequence of length $d - 2a$ into blocks of length 1 (the s's) and 2 (the S's).

For each $K \in sh(a, d - 4a)$, let $\mathcal{F}^K_n \subset \mathcal{F}^d_{n,d-2a}$ be the *shuffle subspace* spanned by monomials of total weight n and of the form of K, where each S represents an element of $\mathcal{S}$ and each s a single s_i. We write $\mathcal{L}$ for the lattice of subspaces of $\mathcal{F}$ generated by the $\mathcal{F}^K_n$; in other words, $\mathcal{L}$ is the set of subspaces $\mathcal{F}^K_n$ and all subspaces obtained from them by sums and intersections.

EXAMPLE 4.3. In the case $n = 24$, $a = 1$ and $d = 6$ as in the example above, we have the decomposition according to the shuffle set $sh(a, d - 4a) = sh(1, 2) = \{Sss, sSs, ssS\}$, so

$$\mathcal{F}^6_{24,4} = \mathcal{F}^{Sss}_{24} + \mathcal{F}^{sSs}_{24} + \mathcal{F}^{ssS}_{24},$$

where

$$\begin{cases} \mathcal{F}^{ssS}_{24} = \langle s_3s_9S_{12}, s_5s_7S_{12}, s_7s_5S_{12}, s_9s_3S_{12}, s_3s_5S_{16}, s_5s_3S_{16}, s_3s_3S_{18}\rangle, \\ \mathcal{F}^{sSs}_{24} = \langle s_3S_{12}s_9, s_5S_{12}s_7, s_7S_{12}s_5, s_9S_{12}s_3, s_3S_{16}s_5, s_5S_{16}s_3, s_3S_{18}s_3\rangle, \\ \mathcal{F}^{Sss}_{24} = \langle S_{12}s_3s_9, S_{12}s_5s_7, S_{12}s_7s_5, S_{12}s_9s_3, S_{16}s_3s_5, S_{16}s_5s_3, S_{18}s_3s_3\rangle. \end{cases}$$

In general, since $\mathcal{F}^d_{n,d-2a}$ is precisely spanned by the shuffles of $d-4a$ s's and a S's, we obtain a decomposition into subspaces

$$\mathcal{F}^d_{n,d-2a} = \sum_{K\in sh(a,d-4a)} \mathcal{F}^K_n. \tag{4.1}$$

The sum (4.1) is not always a direct sum; indeed the shuffle spaces $\mathcal{F}^{Sss}_{24}$ and $\mathcal{F}^{ssS}_{24}$ intersect in the one-dimensional subspace $\mathcal{F}^{SS}_{24}$ generated by S^2_{12} (see Example 4.1). The last result of this section, Proposition 4.6, determines these intersections precisely. To state it, we first need one more definition.

Definition 4.4. Let $K_i \in sh(a_i, d_i-4a_i)$, $i=1,\dots,r$, be shuffles of a_i S's with d_i-4a_i s's, and assume that the numbers d_i-2a_i are all equal to some fixed number $k>0$. The family $K_1,\dots,K_r$ is said to be *compatible* if there exists a shuffle $\mathbf{K}$, called the *intersection* $\mathbf{K}=\cap K_i$ of the K_i, such that each K_i can be obtained from $\mathbf{K}$ by repeating the operation of replacing an S by ss, and $\mathbf{K}$ is the unique shuffle having this property and containing a maximal number of S's.

An equivalent way to define the notions of compatibility and intersection (which justifies the use of the term "intersection") is the following. For $i=1,\dots,r$, let K'_i be the word with k letters obtained from K_i by substituting a double symbol, say TT, for each S. Let B be the set of pairs $(b,b+1)$ of indices, with $1\le b\le d-2a-1$, that index pairs of TT coming from a single S in any of the K_i. Then the family is compatible if the set B consists of disjoint pairs. If so, let $\mathbf{K}'$ be the word in k letters such that all pairs of letters indexed by pairs in B are T's and the rest are s's. By definition, the T's appear in strings of even length in $\mathbf{K}'$, and the intersection $\mathbf{K}$ is obtained from $\mathbf{K}'$ by replacing adjacent pairs of TT by S, starting from the left. If the family is not compatible, we set the intersection $\mathbf{K}=\emptyset$.

Example 4.5. The shuffles $ssSssSs, SssssSs$ and $SSsssss \in sh(2,5)$ form a compatible family, since all can be obtained from $\mathbf{K}=SSssSs$ by replacing one S by ss; the associated words in s,T are $ssTTssTTs$, $TTssssTTs$ and $TTTTsssss$, so $B=\{(3,4),(7,8),(1,2)\}$, $\mathbf{K}'=TTTTssTT$ and $\mathbf{K}=SSssSs$. The shuffles Sss and sSs are not compatible (associated $B=\{(1,2),(2,3)\}$ with common member 2), nor are $sSssssS$ and $sSSSs$ ($B=\{(2,3),(7,8),(4,5),(6,7)\}$ with common member 7). In terms of the ordered partitions into blocks of length 1 or 2 discussed earlier, a compatible family can be viewed as having a common refinement partition of that type.

Proposition 4.6. *Fix $d,a\ge 0$ with $d\ge 4a$. Let $K_1,\dots,K_r$ be distinct shuffles in the shuffle set $sh(a,d-4a)$, and let $\mathbf{K}$ denote their intersection. We write $\mathcal{F}^{\mathbf{K}}_n=\{0\}$ if $\mathbf{K}=\emptyset$. Then*

$$\mathcal{F}^{K_1}_n\cap\cdots\cap\mathcal{F}^{K_r}_n = \mathcal{F}^{\mathbf{K}}_n\,. \tag{4.2}$$

Proof. We use induction on r. If $r=1$ the spaces are identical. Let $\mathbf{H}$ be the intersection of $K_2,\dots,K_r$, and assume that $\cap_{i=2}^r\mathcal{F}^{K_i}_n=\mathcal{F}^{\mathbf{H}}_n$. The two shuffles K_1 and $\mathbf{H}$ form a two-member family whose intersection is still $\mathbf{K}$. By an abuse of notation, let us write $K_2=\mathbf{H}$ and $\mathbf{H}\in sh(a_2,d_2-2a_2)$ (even if these are not the same a_2,d_2 as before), so that $\mathbf{K}$ is the intersection of K_1 and K_2. Thus we only have to prove that $\mathcal{F}^{K_1}_n\cap\mathcal{F}^{K_2}_n=\mathcal{F}^{\mathbf{K}}_n$.

Let V denote the vector space generated by the s_i, and R the vector space generated by the $S\in\mathcal{S}$, so $R\subset V\otimes V$. Then the shuffle spaces $\mathcal{F}^{K_i}$ are equal to the corresponding tensor products of V and R with s replaced by V and S by R. For example, if $K_1 = ssSsss$ and $K_2 = SsssS$, we have

$$\begin{cases} \mathcal{F}^{ssSsss} = V \otimes V \otimes R \otimes V \otimes V \otimes V \\ \mathcal{F}^{SsssS} = R \otimes V \otimes V \otimes V \otimes R. \end{cases}$$

In the case where K_1 and K_2 are compatible families, this precisely means that the two tensor products can be "lined up" in such a way that each R in either $\mathcal{F}^{K_1}$ or $\mathcal{F}^{K_2}$ lines up over either an R or a $V \otimes V$ in the other space. In the example above, which is compatible, we illustrate it by bracketing factors $V \otimes V$ in each tensor product that line up over an R in the other one.

$$\begin{cases} \mathcal{F}^{ssSsss} = \big(V \otimes V\big) \otimes R \otimes V \otimes \big(V \otimes V\big) \\ \mathcal{F}^{SsssS} = R \otimes \big(V \otimes V\big) \otimes V \otimes R. \end{cases}$$

Then since $R \subset V \otimes V$, the intersection of the two spaces is obtained from either one of the two tensor products by replacing $V \otimes V$ by R for each factor of $V \otimes V$ that lines up with an R in the other one. Thus, in the example above, the intersection is $R \otimes R \otimes V \otimes R$. But this is nothing other than the tensor product of V's and R's corresponding to $\mathcal{F}^{\mathbf{K}}$ with $\mathbf{K} = K_1 \cap K_2$ (indeed, in the example, $\mathbf{K} = SSsS$).

In the case where K_1 and K_2 are non-compatible, this means that it is impossible to line up each R in one factor with a $V \otimes V$ in the other; at some point from left to right, this line-up must fail. This means that moving from left to right, at some point in the line-up we must have a factor of $V \otimes R$ in one of the tensor products lying above a factor of $R \otimes V$ in the other. Thus, to prove that $\mathcal{F}^{K_1} \cap \mathcal{F}^{K_2} = \{0\}$, it is enough to show that $V \otimes R \cap R \otimes V = \{0\}$. This is not always true for general vector spaces with $R \subset V \otimes V$, and is quite difficult to show in the present case, but it was proven by Goncharov ([**13**], Theorem 1.5), see also [**8**], Prop. 5.4. □

5. Proof of Theorem 3.4.

Proof of theorem 3.4. (i) To show that $\mathcal{F}^d_{n,k} = \mathcal{F}^{d+1}_{n,k}$ if $k \not\equiv d$ mod 2, it suffices to consider what elements of $\mathcal{F}$ can exist which are of standard depth k and special depth d. The space $\mathcal{F}_{n,k} = \mathcal{F}^k_{n,k}$ is generated by products $s_{i_1} \cdots s_{i_k}$ with $i_1 + \cdots + i_k = n$. By definition, the only elements in $\mathcal{F}^k_{n,k}$ which have special depth $> k$ are those in the intersection of $\mathcal{F}^k_{n,k}$ with the ideal of $\mathcal{F}$ generated by the "special elements" (elements of $\mathcal{S}$); thus they are linear combinations of products of a special elements and c single s_i's. Such a product is of standard depth $k = 2a + c$ and special depth $d = 4a + c$, so $d = 2a + k$, so $d \equiv k$ mod 2. This proves (i).

(ii) The subspace decomposition (4.1) together with Conjecture 3.1 positing the distributivity property of the lattice $\mathcal{L}$ ensures that we may compute the dimension of $\mathcal{F}^d_{n,d-2a}$ via the standard inclusion-exclusion formula:

$$\dim(\mathcal{F}^d_{n,d-2a}) = \dim\Big(\sum_{K \in sh(a,d-4a)} \mathcal{F}^K_n\Big) \tag{5.1}$$

$$= \sum_K \dim\big(\mathcal{F}^K_n\big) - \frac{1}{2!} \sum_{K_1,K_2} \dim\big(\mathcal{F}^{K_1}_n \cap \mathcal{F}^{K_2}_n\big) + \frac{1}{3!} \sum_{K_1,K_2,K_3} \dim\big(\mathcal{F}^{K_1}_n \cap \mathcal{F}^{K_2}_n \cap \mathcal{F}^{K_3}_n\big) - \cdots$$

Indeed, the distributivity of the lattice $\mathcal{L}$ is equivalent to the existence of a basis $\mathcal{B}$ for $\mathcal{F}$ such that $\mathcal{B}\cap\mathcal{F}_n^K$ forms a basis of $\mathcal{F}_n^K$.

We do the computation using the following three lemmas (the proofs of the second and third, somewhat technical, are relegated to §6).

Lemma 5.1. *Fix $d\geq 4a$. Then the dimension of $\mathcal{F}_n^K$ is independent of the shuffle $K\in sh(a,d-4a)$, and is given by the coefficient*

$$\dim(\mathcal{F}_n^K)=(S^aO^{d-4a}|X^n).$$

Proof. The rational function $S(X)$ is the generating series whose coefficients determine the dimensions of the spaces of special elements $\mathcal{S}_m$, and the rational function $O(X)$ is the generating series whose coefficients determine the dimensions of the spaces generated by monomials in the s_i. In other words, $(S(X)^a|X^n)$ determines the dimension of the space of products of a special elements of total weight n, and $(O(X)^b|X^n)$ determines the dimension of the space of products of b s_i of total weight n. Clearly the dimension of $\mathcal{F}_n^K$ is independent of the actual choice of $K\in sh(a,d-4a)$; for each K, the number of monomials is identical, corresponding simply to inserting the a special elements in different positions among the $d-2a$ single s_i. Thus to determine the dimension of $\mathcal{F}_n^K$, we may assume that

$$K=\underbrace{S\cdots S}_{a}\underbrace{s\cdots s}_{d-4a},$$

so that $\mathcal{F}_n^K$ is spanned by monomials $S^1\cdots S^a s^1\cdots s^{d-2a}$. The rational function $S(X)^aO(X)^{d-4a}$ describes exactly the number of these monomials in each weight n. □

Lemma 5.2. *Fix a and d with $d\geq 4a$, and fix $b\geq 1$. Then the number of compatible ordered families $K_1,\ldots,K_r$ of pairwise distinct shuffles in $sh(a,d-4a)$ such that the intersection $\mathbf{K}$ lies in $sh(a',d'-4a')$ with $a'=a+b$ and $d'=d+2b$ is given by*

$$S_{a,b}(r)=\binom{d-3a-b}{a+b}r!\Biggl(\sum_{j=0}^{b}(-1)^j\binom{a+b}{j}\binom{\binom{a+b-j}{a}}{r}\Biggr).$$

Lemma 5.3. *The expressions $S_{a,b}(r)$ from Lemma 5.2 satisfy:*

$$\sum_{r=1}^{\binom{a+b}{a}}(-1)^{r-1}\frac{S_{a,b}(r)}{r!}=(-1)^b\binom{d-3a-b}{a+b}\binom{a+b-1}{b}. \tag{5.2}$$

Let us now use these to complete the proof of Theorem 3.4 by calculating the dimensions from (5.1). Note that the result of Lemma 5.2 shows in particular that

$$b>[(d-4a)/2]\Rightarrow S_{a,b}(r)=0, \tag{5.3}$$

since the binomial coefficient $\binom{d-3a-b}{a+b}$ is zero for such b, and similarly, that

$$r>\binom{a+b}{a}\Rightarrow S_{a,b}(r)=0. \tag{5.4}$$

As above, if $K_1,\ldots,K_r$ form a compatible family, we write $\mathbf{K}$ for the intersection, but if they do not form a compatible family, we set $\mathbf{K}=\emptyset$; then we write

$\mathcal{F}^{\emptyset} = \{0\}$. If the family is compatible, then there exists some $b \geq a$ such that $\mathbf{K} \in sh(a', d'-4a')$ with $a' = a+b$, $d' = d+2b$; in this case, by Lemma 5.1 above, we have

$$\dim(\mathcal{F}_n^{\mathbf{K}}) = (S^{a'}O^{d'-4a'}|X^n) = (S^{a+b}O^{d-4a-2b}|X^n). \tag{5.5}$$

We now fix $d, a \geq 0$ with $d \geq 4a$, and a weight n such that $n \geq 3d$.

The preceding results give us a way to compute the dimensions of the key intersections that we need to calculate $\dim(\mathcal{F}^d_{n,d-2a})$ using (5.1).

We rewrite (5.1) in terms of shuffles $K \in sh(a, d-4a)$ as:

$$\begin{aligned}
\dim(\mathcal{F}^d_{n,d-2a}) &= \dim\Big(\sum_K \mathcal{F}_n^K\Big) \\
&= \sum_{r\geq 1}(-1)^{r-1}\frac{1}{r!}\sum_{K_1,\ldots,K_r} \dim\big(\mathcal{F}_n^{K_1}\cap\cdots\cap\mathcal{F}_n^{K_r}\big) \\
&= \sum_{r\geq 1}(-1)^{r-1}\frac{1}{r!}\sum_{b=1}^{[(d-4a)/2]}\ \sum_{\substack{K_1,\ldots,K_r\ s.t.\\ \mathbf{K}\in sh(a+b,d-4a-2b)}} \underbrace{\dim\big(\mathcal{F}_n^{K_1}\cap\cdots\cap\mathcal{F}_n^{K_r}\big)}_{=\underbrace{\dim(\mathcal{F}_n^{\mathbf{K}})}_{=(S^{a+b}O^{d-4a-2b}|X^n)\quad \text{by } (5.5)}\quad \text{by } (4.2)} \quad \text{by } (5.3) \\
&= \sum_{r\geq 1}(-1)^{r-1}\frac{1}{r!}\sum_{b=1}^{[(d-4a)/2]} S_{a,b}(r)(S^{a+b}O^{d-4a-2b}|X^n) \quad \text{by Lemma 5.8} \\
&= \sum_{b=1}^{[(d-4a)/2]}\Bigg(\sum_{r=1}^{\binom{a+b}{a}}(-1)^{r-1}\frac{1}{r!}S_{a,b}(r)\Bigg)(S^{a+b}O^{d-4a-2b}|X^n) \quad \text{by } (5.4) \\
&= \sum_{b=1}^{[(d-4a)/2]}(-1)^b\binom{d-3a-b}{a+b}\binom{a+b-1}{b}(S^{a+b}O^{d-4a-2b}|X^n) \quad \text{by } (5.2).
\end{aligned}$$

Setting $c = d-4a-2b$, we rewrite this formula as

$$\dim(\mathcal{F}^d_{n,d-2a}) = \sum_{\substack{2b+c=d-4a\\ b,c\geq 0}}(-1)^b\binom{a+b+c}{c}\binom{a+b-1}{b}(S^{a+b}O^c|X^n). \tag{5.6}$$

Applying (5.6) to the situation (d, a) and also $(d+2, a+1)$ for the same n and taking the difference, and using the standard binomial identity $\binom{k}{j} = \binom{k-1}{j} + \binom{k-1}{j-1}$, we immediately obtain

$$\dim(\mathcal{F}^d_{n,d-2a}/\mathcal{F}^{d+2}_{n,d-2a}) = \sum_{\substack{2b+c=d-4a\\ b,c\geq 0}}(-1)^b\binom{a+b+c}{c}\binom{a+b}{b}(S^{a+b}O^c|X^n). \tag{5.7}$$

To conclude the proof of Theorem 3.4, we show that

$$\sum_{\substack{2b+c=d-4a\\ b,c\geq 0}}(-1)^b\binom{a+b+c}{c}\binom{a+b}{b}(S^{a+b}O^c|X^n) = e^d_{n,d-2a},$$

the coefficient of the monomial $X^nY^{d-2a}Z^d$ in the three-variable Broadhurst-Kreimer function. The Taylor expansion of this function in Y and Z is given by

$$\sum_{k\geq 0}(SY^2Z^4 - SY^2Z^2 + OYZ)^k. \tag{5.8}$$

Using the standard formula for expanding trinomials

$$(x+y+z)^k = \sum_{a+b+c=k}\binom{a+b+c}{a,b}x^ay^bz^c,$$

where

$$\binom{a+b+c}{a,b} = \frac{(a+b+c)!}{a!\,b!\,c!},$$

we find that the monomial $Y^{d-2a}Z^d$ appears in in (5.8) as

$$\sum_{\substack{4A+2B+C=d\\ C+2B+2A=d-2a}} \binom{A+B+C}{A,B}(SY^2Z^4)^A(-SY^2Z^2)^B(OYZ)^C =$$

$$\sum_{\substack{4A+2B+C=d\\ C+2B+2A=d-2a}} (-1)^B\binom{A+B+C}{A,B}S^{A+B}O^CY^{C+2B+2A}Z^{C+2B+4A}$$

$$\sum_{2B+C=d-4a} (-1)^B\binom{a+B+C}{a,B}O^CS^{a+B}Y^{d-2a}Z^d.$$

Replacing B, C by b, c and using the identity of binomial and trinomial coefficients

$$\binom{a+b+c}{c}\binom{a+b}{b} = \binom{a+b+c}{a,b}$$

completes the proof of Theorem 3.4. ☐

6. Proofs of Lemmas 5.2 and 5.3.

Proof of lemma 5.2. Though a little complicated, this lemma is proved by the same basic inclusion-exclusion technique as in formula (5.1). Consider the set of all compatible families of r shuffles $K_1,\ldots,K_r \in sh(a, d-4a)$ whose intersection $\mathbf{K}$ lies in $sh(a', d'-4a')$ with $a' = a+b$, $d' = d+2b$. Since $\mathbf{K}$ is a shuffle of $a' = a+b$ S's with $d'-4a' = d-4a-2b$ s's, there are exactly $\binom{d-3a-b}{a+b}$ possibilities for $\mathbf{K}$.

The statement of the lemma is now reduced to the claim that the number of compatible r-families $K_1,\ldots,K_r \in sh(a, d-4a)$ whose intersection $\mathbf{K}$ is a *fixed* element of $sh(a+b, d-4a-2b)$ is equal to $r!$ (corresponding to all possible orders of a given unordered family $\{K_1,\ldots,K_r\}$) times

$$\sum_{j=0}^{b}(-1)^j\binom{a+b}{j}\binom{\binom{a+b-j}{a}}{r}. \tag{6.1}$$

In the word $\mathbf{K}$ in letters s and S, whose total number of letters is $d-3a-b$, let $p_1,\ldots,p_{a+b}$ denote the positions of the $a+b$ letters S. Since $\mathbf{K}$ is the intersection of the K_i, each K_i can be obtained from $\mathbf{K}$ by replacing exactly b S's in $\mathbf{K}$ by ss, leaving a S's intact. Let $\{p_1,\ldots,p_{a+b}\} \subset \{1,\ldots,d-3a-b\}$ denote the indices of the letters S in the word $\mathbf{K}$. Thus, the number of families $K_1,\ldots,K_r$ with intersection $\mathbf{K}$ is the same as the number of families of r subsets of order a of $\{p_1,\ldots,p_{a+b}\}$ whose union covers $\{p_1,\ldots,p_{a+b}\}$; this is the same as asking for families of r subsets of order a of $\{1,\ldots,a+b\}$ whose union covers $\{1,\ldots,a+b\}$. Thus, we may identify each K_i with a subset of order a of $\{1,\ldots,a+b\}$.

The total number of families of r subsets of order a of $\{1,\ldots,a+b\}$ is given by

$$\binom{\binom{a+b}{a}}{r}. \tag{6.2}$$

From this we have to subtract off the number of "bad" families, those whose union does not cover the whole set $\{1,\ldots,a+b\}$.

For any family $K_1,\ldots,K_r$ that does not cover, its intersection $\mathbf{K}$ must necessarily be contained in one of the $a+b$ subsets of $\{1,\ldots,a+b\}$ of order $a+b-1$. Let $R_1,\ldots,R_{a+b}$ denote these subsets, and for $1\le i\le a+b$, let $\mathcal{R}_i$ denote the collection of "bad" families of order r whose union lives inside R_i. The bad families are thus those in the union $\mathcal{R}_1\cup\cdots\cup\mathcal{R}_{a+b}$. To compute the order of this union, we use the inclusion-exclusion formula

$$|\mathcal{R}_1\cup\cdots\cup\mathcal{R}_{a+b}|=\sum_{j=1}^{a+b}(-1)^{j-1}\sum_{1\le i_1<\cdots<i_j\le a+b}|\mathcal{R}_{i_1}\cap\cdots\cap\mathcal{R}_{i_j}|.$$

But the intersection $\mathcal{R}_{i_1}\cap\cdots\cap\mathcal{R}_{i_j}$ is just the set of families which live in the subset $R_{i_1}\cap\cdots\cap R_{i_j}$, which is of order $a+b-j$, so

$$|\mathcal{R}_{i_1}\cap\cdots\cap\mathcal{R}_{i_j}|=\binom{\binom{a+b-j}{a}}{r},$$

which vanishes when $j>b$, so the number of bad families is equal to

$$|\mathcal{R}_1\cup\cdots\cup\mathcal{R}_{a+b}|=\sum_{j=1}^{a+b}(-1)^{j-1}\sum_{1\le i_1<\cdots<i_j\le a+b}\binom{\binom{a+b-j}{a}}{r}=\sum_{j=1}^{b}(-1)^{j-1}\binom{a+b}{j}\binom{\binom{a+b-j}{a}}{r}. \tag{6.3}$$

Thus, the number of good families is given by the difference between (6.2) and (6.3), which is precisely equal to (6.1). This proves the lemma. □

Proof of lemma 5.3. The statement comes down to proving that

$$\sum_{r=1}^{\binom{a+b}{a}}(-1)^{r-1}\sum_{j=0}^{b}(-1)^j\binom{a+b}{j}\binom{\binom{a+b-j}{a}}{r}=(-1)^b\binom{a+b-1}{b}.$$

By switching the sums and removing the zero terms, we write this as

$$\sum_{j=0}^{b}(-1)^j\binom{a+b}{j}\sum_{r=1}^{\binom{a+b-j}{a}}(-1)^{r-1}\binom{\binom{a+b-j}{a}}{r}=(-1)^b\binom{a+b-1}{b}.$$

Written this way, it is clear that the inner sum over r is equal to 1, so the equality becomes

$$\sum_{j=0}^{b}(-1)^j\binom{a+b}{j}=(-1)^b\binom{a+b-1}{b}.$$

This identity follows easily from the standard identities

$$\binom{m}{n}=\sum_{k=0}^{n}\binom{m-n-1+k}{k},$$

together with

$$\binom{-a}{b} = (-1)^b \binom{a+b-1}{b}.$$

□

7. Multiple zeta values and their duals

In this final section, we explain the relation between our main theorem and the theory of multiple zeta values, whether formal, motivic or real. We keep the exposition as brief as possible, however we do need to introduce a certain number of well-known facts and properties concerning multiple zeta values. The goal is to explain what we see as the meaning of the Broadhurst-Kreimer dimension conjecture, and relate it to the results of Theorem 3.3 on the dimensions of $\mathcal{F}_n^d$.

7.1. Real and formal multiple zeta values.

DEFINITION 7.1. The *multiple zeta algebra* $\mathcal{Z}$ is generated over $\mathbb{Q}$ by the real numbers known as *multiple zeta values*, given by

$$\zeta(k_1,\ldots,k_d) = \sum_{n_1>\cdots>n_d>0} \frac{1}{n_1^{k_1}\cdots n_d^{k_d}}, \tag{7.1}$$

where the k_i are strictly positive integers, with $k_1 > 1$ in order to ensure convergence of the series, and $k_1+\cdots+k_d \geq 2$. The number d is the *y-depth* of the multiple zeta value, and its weight n is given by $k_1+\cdots+k_d = n$. We let $\overline{\mathcal{Z}}$ denote the quotient of $\mathcal{Z}$ modulo the ideal generated by $\zeta(2)$; this is the *reduced* multiple zeta algebra.

Let $\mathcal{Z}_n^d$ denote the vector space over $\mathbb{Q}$ spanned by multiple zeta values of weight n and y-depth d, and let $\overline{\mathcal{Z}}_n^d$ denote its image in $\overline{\mathcal{Z}}$. The Broadhurst-Kreimer function was first identified by Broadhurst and Kreimer [**3**] when they used a computer to calculate the dimensions of the subspace $\overline{\mathcal{Z}}_n^d$ modulo $\overline{\mathcal{Z}}_n^{d-1}$ for quite high values of n and d (it has successively been corroborated numerically considerably further by Bluemlein, Broadhurst and Vermaseren [**2**]); they realized that these dimensions formed the coefficients of the Taylor series of $BK(X,Y)$ (cf. (1.1)), and conjectured that $BK(X,Y)$ yields the correct dimensions for all n,d, i.e. that

$$c_n^d = \overline{\mathcal{Z}}_n^d/\overline{\mathcal{Z}}_n^{d-1} \tag{7.2}$$

for $n \geq 3$, $d \geq 1$, where c_n^d is the coefficient of X^nY^d in $BK(X,Y)$.

In particular, the function $BK(X,1)$ then conjecturally determines the dimensions of the weight n subspaces $\overline{\mathcal{Z}}_n$. It is obviously not known whether the weight forms a grading of $\mathcal{Z}$ or $\overline{\mathcal{Z}}$ – indeed, not much is known even about the transcendence of the single zeta values $\zeta(n)$ for odd $n \geq 3$ – but the conjecture implies that the weight is indeed a grading, and that the dimensions of $\overline{\mathcal{Z}}_n$ are given by the generating series

$$BK(X,1) = (1-X^2)/(1-X^2-X^3) \tag{7.1}$$

first observed by Zagier [**25**], [**26**].

We now need to introduce some basic notions. Define the *shuffle product* of words in non-commutative variables x,y recursively by the formula

$$sh(u,1) = sh(1,u) = u,$$

$$sh(Xu, Yv) = X \cdot sh(u, Yv) + Y \cdot sh(Xu, v),$$

where $X, Y \in \{x, y\}$. We write $\mathrm{Lie}_n[x, y]$ for the vector space of weight n (i.e. degree n) Lie polynomials. For any polynomial $f \in \mathbb{Q}\langle x, y\rangle$, let $(f|w)$ denote the coefficient of a word w in the polynomial f, and extend it linearly, i.e. $(f|au+bv) = a(f|u) + b(f|v)$. It is a well-known fact that for a polynomial $f \in \mathbb{Q}\langle x, y\rangle$, we have

$$f \in \mathrm{Lie}[x, y] \;\Leftrightarrow\; \big(f|sh(u, v)\big) = 0 \;\text{ for all words } u, v \text{ in } x, y. \tag{7.2}$$

We define the *stuffle product* of words in x, y ending in y as follows. Set $y_i = x^{i-1}y$ for $i \geq 1$; all words ending in y can be written $y_{i_1} \cdots y_{i_r}$. We define the stuffle product of two such words by

$$st(v, 1) = st(1, v) = v,$$

$$st(y_{i_1}y_{i_2}\cdots y_{i_r}, y_{j_1}y_{j_2}\cdots y_{j_s}) = y_{i_1} \cdot st(y_{i_2}\cdots y_{i_r}, y_{j_1}y_{j_2}\cdots y_{j_s})$$
$$+y_{j_1} \cdot st(y_{i_1}y_{i_2}\cdots y_{i_r}, y_{j_2}\cdots y_{j_s}) + y_{i_1+j_1} \cdot st(y_{i_2}\cdots y_{i_r}, y_{j_2}\cdots y_{j_r}).$$

We say that a word is convergent if it starts in x and ends in y. Any convergent word can be written $w = y_{k_1}\cdots y_{k_d}$ with $k_1 > 1$; we set $\zeta(w) = \zeta(k_1, \ldots, k_d)$. Following [**9**], we extend the definition of $\zeta(w)$ from convergent words to all words in x, y by the following formula. If w is not convergent, write $w = y^a u x^b$ where u is convergent; then set

$$\zeta(w) = \sum_{r=0}^{a}\sum_{s=0}^{b}(-1)^{a+b}\zeta\Big(\pi\big(sh(y^r, y^{a-r}ux^{b-s}, x^s)\big)\Big), \tag{7.3}$$

where ζ is considered to be linear on words, and π denotes the projector sending a polynomial onto only its part consisting of convergent words (and $sh(w_1, w_2, w_3)$ is defined as $sh\big(w_1, sh(w_2, w_3)\big)$).

We also define a different extension of $\zeta(w)$, this time from convergent words only to words starting and ending in y. We begin by defining values $\zeta_*(\underbrace{1, \ldots, 1}_{n})$ by the equality

$$1 + \sum_{n\geq 1}\zeta_*(\underbrace{1, \ldots, 1}_{n})y^n = \exp\Big(\sum_{n\geq 2}\frac{(-1)^{n-1}}{n}\zeta(x^{n-1}y)y^n\Big).$$

In particular, we have $\zeta_*(1) = \zeta(1) = 0$, $\zeta_*(1, 1) = -\frac{1}{2}\zeta(2)$, $\zeta_*(1, 1, 1) = \frac{1}{3}\zeta(3)$ and $\zeta_*(1, 1, 1, 1, 1) = \frac{1}{5}\zeta(5) - \frac{1}{6}\zeta(3)\zeta(2)$. It is clear from the definition that $\zeta_*(\underbrace{1, \ldots, 1}_{n}) \in \mathcal{Z}$ is always an algebraic expression in the $\zeta(x^{n-1}y)$ for $n \geq 1$.

Now, for any word w starting and ending in y, we write $w = y^k u$ with u convergent, and set

$$\zeta_*(w) = \sum_{i=0}^{k}\zeta_*(\underbrace{1, \ldots, 1}_{i})\zeta(y^{k-i}u).$$

Again, the $\zeta_*(w)$ are all algebraic expressions in the $\zeta(w)$.

It is a well-known and fundamental result of the theory of multiple zeta values that the $\bar{\zeta}$ and $\bar{\zeta}_*$ satisfy the following two families of algebraic relations:

(Regularized) shuffle relation: For any two words u and v in x, y,

$$\zeta\big(sh(u, v)\big) = \zeta(u)\zeta(v). \tag{7.4}$$

(Regularized) stuffle relation: Let W_y denote the set of words in x, y ending in y. Then for all $u, v \in W_y$,

$$\zeta_*\big(st(u,v)\big) = \zeta_*(u)\zeta_*(v). \tag{7.5}$$

Definition 7.2. Let $\mathcal{FZ}$ denote the $\mathbb{Q}$-algebra generated by formal symbols $Z(w)$ for all words w in x, y, subject to the relations above. For any convergent word w, we again write $w = y_{k_1} \cdots y_{k_d}$ and $Z(k_1, \ldots, k_d) = Z(w)$.

This $\mathcal{FZ}$ is called the *formal multiple zeta algebra*, and it is one of the major conjectures in the theory of multiple zeta values that $\mathcal{FZ} \simeq \mathcal{Z}$. Obviously $\mathcal{FZ}$ surjects onto $\mathcal{Z}$ since the real multizeta values are known to satisfy (7.4) and (7.5) but the injectivity seems out of reach for the present. To give an idea of the difficulty of this conjecture, it would imply in particular that the weight n gives a grading on $\mathcal{Z}$, which in turn would imply that all multiple zeta values are transcendental (indeed, if a non-zero multiple zeta value is algebraic, then expanding out its minimal polynomial according to (7.4) would give a linear combination of multiple zetas in different weights equal to zero, contradicting the weight grading).

Let $\overline{\mathcal{FZ}}$ be the quotient of $\mathcal{FZ}$ by the ideal generated by $Z(xy) = Z(2)$. It is known that $\overline{\mathcal{FZ}}$ is a Hopf algebra, because it arises as the dual of the enveloping algebra of a Lie algebra (see the next section). It is weight-graded since the relations take place within weight-graded parts. The weight 0 part is given by $\overline{\mathcal{FZ}}_0 = \mathbb{Q}$, then $\overline{\mathcal{FZ}}_1 = \overline{\mathcal{FZ}}_2 = \{0\}$, and $\overline{\mathcal{FZ}}_3 = \{Z(3)\}$.

Following Furusho [**9**], we set $\mathfrak{nfz} = \overline{\mathcal{FZ}}/\mathcal{I}$ where $\mathcal{I}$ is the ideal generated by constants and products, i.e. by $\overline{\mathcal{FZ}}_0$ and $(\overline{\mathcal{FZ}}_{\geq 3})^2$. A priori, $\mathfrak{nfz}$ is simply a vector space, but because it is known that its graded dual is a Lie algebra (again, see next section), it follows that $\mathfrak{nfz}$ has the structure of a weight-graded Lie coalgebra, and that the dimensions of its graded pieces are equal to those of the dual, so that the dimensions of the graded pieces of $\overline{\mathcal{FZ}}$ are equal to those of the universal enveloping algebra of the dual to the Lie coalgebra. We write $z(w)$ for the image in $\mathfrak{nfz}$ of $Z(w) \in \mathcal{FZ}$. It follows from the definitions that for every word w ending in y which is not a power of y, the image of $Z(w)$ is equal to the image of $Z^*(w)$ in $\mathfrak{nfz}$. These $z(w)$ satisfy linearized versions of the double shuffle relations (7.4) and (7.5), namely

$$z\big(sh(u,v)\big) = 0 \tag{7.6}$$

for all pairs of words u, v in x, y, and

$$z\big(st(u,v)\big) = 0 \tag{7.7}$$

for all pairs of words u, v not both powers of y.

7.2. The double shuffle Lie algebra. In this subsection, we give an explicit definition of the *double shuffle* Lie algebra $\mathfrak{ds}$, which is the graded dual of the Lie coalgebra $\mathfrak{nfz}$ of formal multiple zetas defined in the preceding section. The advantage of studying the dual Lie algebra is that its structure can be given more economically in terms of Lie algebra generators, while the dimensions of its graded parts are of course the same as those of $\mathfrak{nfz}$. The definition of $\mathfrak{ds}$ is given by formally dualizing (7.6) and (7.7).

Let W_y denote the set of words ending in y as above, and let W'_y denote the set of pairs (u, v) of words in W_y that are not both powers of y.

Definition 7.3. Let $\mathfrak{ds}$ denote the *double shuffle* Lie algebra defined as follows (7.8)

$$\mathfrak{ds} = \Big\{ f \in \mathbb{Q}_{\geq 3}\langle x, y\rangle \,\Big|\, \big(f|sh(u,v)\big) = 0 \ \ \forall\ u, v,\ \big(f|st(u,v)\big) = 0 \ \ \forall\ (u,v) \in W'_y \Big\},$$

where $\mathbb{Q}_{\geq 3}\langle x, y\rangle$ is the set of polynomials in x, y of degree ≥ 3.

The terminology *double shuffle* comes from the fact that $f \in \mathfrak{ds}$ satisfies the shuffle equations (7.4) and the stuffle equations (7.5). Note that, by (7.2), elements of $\mathfrak{ds}$ lie in $\mathrm{Lie}[x, y]$.

The proof that $\mathfrak{ds}$ is a Lie algebra was discovered by Racinet in his thesis [**21**]. He worked with the Poisson bracket defined as follows: to any $f \in \mathrm{Lie}[x, y]$, associate a derivation D_f of $\mathrm{Lie}[x, y]$ defined by $D_f(x) = 0$, $D_f(y) = [y, f]$. Then $[D_f, D_g] = D_{\{f,g\}}$ where $\{f, g\} = [f, g] + D_f(g) - D_g(f)$. Racinet showed that $\mathfrak{ds}$ is stable under the Poisson Lie bracket defined by $\{\cdot, \cdot\}$ (also called the Ihara bracket). This implies that $\mathcal{U}\,\mathfrak{ds}$ is a Hopf algebra, so its dual $\mathcal{FZ}$ is a Hopf algebra and the quotient by products $\mathfrak{nfz}$ is a Lie coalgebra; in other words, $\mathfrak{nfz}^* \simeq \mathfrak{ds}$.

The Lie algebra $\mathfrak{ds}$ is graded by the weight (i.e. degree) of the Lie polynomials. The first interesting elements, written in the Lyndon-Lie basis, are

$$f_3 = [x, [x, y]] + [y, [x, y]]$$

$$\begin{aligned} f_5 = {} & [x, [x, [x, [x, y]]]] + 2[x, [x, [[x, y], y]]] - \frac{3}{2}[[x, [x, y]], [x, y]] \\ & +2[x, [[[x, y], y], y]] + \frac{1}{2}[[x, y], [x, [x, y]]] + [[[[x, y], y], y], y]. \end{aligned}$$

The dimensions of $\mathfrak{ds}_n$ are equal to 0 for $n = 4, 6$ and to 1 for $n = 3, 5, 7, 8, 9$. Thus there is a canonical generator f_n (up to scalar multiple) for $n = 3, 5, 7, 9$. The Lie algebra $\mathfrak{ds}$ is also equipped with a decreasing *y-depth filtration*, defined by letting the y-depth of a polynomial be equal to the smallest number of y's in any of its monomials. We write $\mathfrak{ds}^1 \supset \mathfrak{ds}^2 \supset \cdots$ for this filtration.

The elements f_n for $n = 3, 5, 7, 9$ are all of y-depth 1. Indeed, it is known (cf. [R]) that for each odd weight $n \geq 3$, there exists an element of y-depth 1 in $\mathfrak{ds}$; y-depth 1 means that the Lie polynomial contains at least one of the Lie words $\mathrm{ad}(x)^i(y)$ with non-zero coefficient. A well-known conjecture states that any choice $f_3, f_5, f_7, \ldots$ of such elements provides a free generating set for $\mathfrak{ds}$.

We relate our work in the previous sections to the theory of multiple zeta values via the following conjecture. Let $\mathrm{Lie}\,\mathcal{F}$ denote the free algebra $\mathrm{Lie}[s_3, s_5, \ldots] \subset \mathcal{F}$. The special depth filtration on $\mathcal{F}$ restricts naturally to one on $\mathrm{Lie}\,\mathcal{F}$.

Conjecture 7.4. *Let $f_3, f_5, \ldots$ be a chosen set of y-depth 1 elements of $\mathfrak{ds}$ in each odd weight ≥ 3. Then the Lie algebra homomorphism*

$$\rho : \mathrm{Lie}\,\mathcal{F} \to \mathfrak{ds} \tag{7.9}$$

mapping $s_i \mapsto f_i$ is a bijection, and furthermore it carries the special depth filtration on $\mathrm{Lie}\,\mathcal{F}$ *to the y-depth filtration on* $\mathcal{U}\,\mathfrak{ds}$.

Thus the conjecture implies that the universal enveloping algebra of $\mathfrak{ds}$, which is dual to the Hopf algebra of formal multiple zeta values $\mathcal{FZ}$, is isomorphic to $\mathcal{F}$, and so our results on the dimensions of the associated graded pieces of $\mathcal{F}$ would lead to

$$\dim \mathcal{U}\,\mathfrak{ds}_n^d / \mathcal{U}\,\mathfrak{ds}_n^{d+1} = c_n^d,$$

where c_n^d is the coefficient of the monomial X^nY^d in the Broadhurst-Kreimer function $BK(X,Y)$. By duality, this would mean that

$$\dim \overline{\mathcal{FZ}}_n^d/\overline{\mathcal{FZ}}_n^{d-1} = c_n^d,$$

which corresponds exactly to Broadhurst-Kreimer's original motivation given in (7.2), except that it would hold for formal multizeta values whereas their original conjecture concerns the real ones.

7.3. Evidence for the conjecture. The Lie algebra $\mathfrak{ds}$ has been calculated explicitly up to about weight 20, and the resulting dimensions bear out the correctness of the Broadhurst-Kreimer dimensions for $\mathfrak{ds}_n^d/\mathfrak{ds}_n^{d+1}$. However, there is also some more theoretical evidence in favor of Conjecture 7.4.

7.3.1. *Injectivity of the homomorphism* $\rho : \mathrm{Lie}\,\mathcal{F} \to \mathfrak{ds}$. Although we do not know much about the Lie homomorphism (7.9) for a general choice of $f_3, f_5, \ldots$ in $\mathfrak{ds}$, we can show that there exist choices of y-depth 1 elements such that ρ is injective. Let us sketch how this is known.

In a series of articles (see e.g. [**17**], but also [**11**], [**15**], [**12**], [**7**]), Goncharov (and co-authors) defined *motivic multiple zeta values*, which are (framed) mixed Tate motives whose associated periods are real multiple zeta values, and which form a Hopf algebra denoted $\mathcal{MZ}$ under the tensor product, with a coproduct defined explicitly by Goncharov ([**12**], foreshadowed by [**11**]). It is known that the motivic multiple zeta values satisfy relations (7.4)–(7.5) (see [**12**], for (7.5) see also [**23**]). Thus there are surjections

$$\overline{\mathcal{FZ}} \to \mathcal{MZ} \to \overline{\mathcal{Z}},$$

where the second surjection comes from taking the period of a framed mixed Tate motive.

In a remarkable paper, Brown [**4**], with help from Zagier [**27**], recently succeeded in proving that the dimensions of the weight graded parts of $\mathcal{MZ}$ are given by the coefficients of the generating series $BK(X,1)$ (cf. (7.1)). Thus, as was pointed out earlier by Goncharov ([**16**], or see 25.7.3.1 of [**1**] for more detail, as well as [**24**]), these dimensions form an upper bound for the dimensions of the weight n parts $\overline{\mathcal{Z}}_n$ of $\overline{\mathcal{Z}}$, and a lower bound for the dimensions of $\overline{\mathcal{FZ}}_n$. Writing $\mathfrak{nmz}$ for the quotient of $\mathcal{MZ}$ by the degree 0 part and products, the surjection $\overline{\mathcal{FZ}} \twoheadrightarrow \mathcal{MZ}$ induces a surjection of quotients $\mathfrak{nfz} \twoheadrightarrow \mathfrak{nmz}$. Thanks to [**21**], Goncharov's coproduct passes to a cobracket on $\mathfrak{nmz}$, which is in fact a Lie coalgebra, so by duality this yields an injection of Lie algebras

$$\mathfrak{nmz}^* \hookrightarrow \mathfrak{nfz}^* = \mathfrak{ds}.$$

It follows directly from Brown's dimension result that the Lie algebra $\mathfrak{nmz}^*$ is free on one y-depth 1 generator for each odd $n \geq 3$.

These observations thus show that there is at least one choice of a set of y-depth 1 elements f_n for odd $n \geq 3$ in $\mathfrak{ds}$ (namely the images of a set of Lie generators for $\mathfrak{nmz}^*$) which generate a free Lie subalgebra inside $\mathfrak{ds}$. Thus, for this choice of f_i, the map (7.9) is injective.

7.3.2. *Compatibility of $\rho : \mathrm{Lie}\,\mathcal{F} \to \mathfrak{ds}$ with the depth filtrations.* There is also some evidence to support the part of Conjecture 7.4 concerning the depth filtrations. Assume that generators f_i are chosen as above, so that ρ is injective.

By the definition of the y-depth filtration, a Poisson bracket of d f_i's lies in $\mathfrak{ds}^d$, so we have maps

$$\rho : \mathrm{Lie}\,\mathcal{F}^i \to \mathfrak{ds}^i$$

for $i = 1, 2, 3$.

Racinet [**21**] proved that $\mathfrak{ds}^1/\mathfrak{ds}^2$ is generated by one element in each odd rank ≥ 3, so the induced map

$$\overline{\rho} : \mathrm{Lie}\,\mathcal{F}^1/\mathrm{Lie}\,\mathcal{F}^2 \to \mathfrak{ds}^1/\mathfrak{ds}^2$$

is an isomorphism.

In y-depth 2, it was shown in [**22**] that the only relations in $\mathfrak{ds}^2/\mathfrak{ds}^3$ between (images of) double Poisson brackets $\{f_i, f_j\}$ are of the form

$$\sum_{i,j} a_{ij}\{f_i, f_j\} \equiv 0 \quad \text{modulo} \quad \mathfrak{ds}^3, \tag{7.10}$$

where $\sum_{i,j} a_{ij}(X^{i-1}Y^{j-1} - X^{j-1}Y^{i-1})$ is a reduced even period polynomial. Thus the definition of the special depth filtration shows that

$$\overline{\rho} : \mathrm{Lie}\,\mathcal{F}^2/\mathrm{Lie}\,\mathcal{F}^3 \to \mathfrak{ds}^2/\mathfrak{ds}^3$$

is an isomorphism.

In y-depth 3, a combination of impressive dimension results due to Goncharov [**14**] with Brown's theorem mentioned above shows that $\mathfrak{ds}^3$ is generated by triple Poisson brackets $\{f_i, \{f_j, f_k\}\}$ and that the induced map

$$\overline{\rho} : \mathrm{Lie}\,\mathcal{F}^3/\mathrm{Lie}\,\mathcal{F}^4 \to \mathfrak{ds}^3/\mathfrak{ds}^4$$

is also an isomorphism.

The interesting phenomenon starts in y-depth 4. Naturally, the relations (7.10) give rise to many relations of higher y-depth in $\mathfrak{ds}$ by bracketing; for example the period polynomial (2.1) corresponds to $\{f_3, f_9\} - 3\{f_5, f_7\}$, and we also have the relation

$$\{f_3, \{f_3, f_9\}\} - 3\{f_3, \{f_5, f_7\}\} \equiv 0 \;\; \text{modulo} \;\; \mathfrak{ds}^4.$$

In fact, it is known ([**18**]) that the "period-polynomial elements" (7.10) lie not just in $\mathfrak{ds}^3$ but in $\mathfrak{ds}^4$. Conjecture 7.4 is tantamount to assuming that (i) these period-polynomial elements lie in $\mathfrak{ds}^4$ and are non-zero modulo $\mathfrak{ds}^5$, and (ii) all relations in the associated graded of $\mathfrak{ds}$ for the y-depth filtration come from the Lie ideal of $\mathfrak{ds}$ generated by the relations (7.10). In [**5**], Brown considers similar questions relating this type of assertion to the Broadhurst-Kreimer function, but rather than with $\mathrm{Lie}\,\mathcal{F}$ and $\mathfrak{ds}$, he works with the Lie algebra $\mathfrak{nmz}$ and another Lie algebra, called "linearized double shuffle", which is known to contain the associated graded of $\mathfrak{ds}$.

Because the period polynomial elements lie in $\mathfrak{ds}^4$, the map ρ sends $\mathrm{Lie}\,\mathcal{F}^4 \to \mathfrak{ds}^4$. In order for the induced map $\overline{\rho} : \mathrm{Lie}\,\mathcal{F}^4/\mathrm{Lie}\,\mathcal{F}^5 \to \mathfrak{ds}^4/\mathfrak{ds}^5$ to be an isomorphism, we would need to know (i) and (ii) above in y-depth 4, i.e. that the period polynomial elements are not in the kernel, and that there are no relations in $\mathfrak{ds}^4/\mathfrak{ds}^5$ other than those coming from the Lie ideal generated by the period polynomial elements.

Although we do not know either of these facts at present, it is at least easy to show that for each period polynomial, there does exist a choice of free y-depth 1 generators $f_3, f_5, \ldots$ of the motivic Lie subalgebra $\mathfrak{nmz}^*$ in $\mathfrak{ds}$ such that the period-polynomial element in those generators is non-zero in $\mathfrak{ds}^4/\mathfrak{ds}^5$. Indeed, if we had

$$\sum_{\substack{i<j\\ i+j=n}} a_{ij}\{f_i, f_j\} \in \mathfrak{ds}_n^5$$

for a given choice of f_k's, it would be sufficient to pick the smallest i such that a_{ij} is non-zero, and change $f_j = f_{n-i}$ to $f_j + \{f_a, \{f_b, f_c\}\}$ with $a+b+c=j$. Such triple brackets exist as soon as $j \geq 11$. Since $i<j<11$, the only possibilities are $(i,j) = (3,5), (3,7), (3,9), (5,7), (5,9), (7,9)$ in weights 8,10,12,14,16. There are no period polynomials in weights 8,10 and 14, and only one up to scalar multiple in each of weights 12 and 16; the corresponding period polynomial elements in $\mathfrak{ds}$ can be calculated explicitly, and it turns out that they do not vanish in $\mathfrak{ds}^4/\mathfrak{ds}^5$. Thus, this method yields at least the partial result that for each period polynomial, there exists a choice of motivic generators $f_3, f_5, \ldots$, such that the corresponding period polynomial element does not vanish in $\mathfrak{ds}^4/\mathfrak{ds}^5$. It would be very helpful to prove that this result holds independently of the choice of motivic generators f_n.

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