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Mixed Tate motives over $\mathbb{Z}$

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Abstract

We prove that the category of mixed Tate motives over $\mathbb{Z}$ is spanned by the motivic fundamental group of $\mathbb{P}^1$ minus three points. We prove a conjecture by M. Hoffman which states that every multiple zeta value is a $\mathbb{Q}$-linear combination of $\zeta(n_1, \ldots, n_r)$, where $n_i \in \{2, 3\}$.

1. Introduction

Let $\mathcal{MT}(\mathbb{Z})$ denote the category of mixed Tate motives unramified over $\mathbb{Z}$. It is a Tannakian category with Galois group $\mathcal{G}_{\mathcal{MT}}$. Let $\mathcal{MT}'(\mathbb{Z})$ denote the full Tannakian subcategory generated by the motivic fundamental group of $\mathbb{P}^1\backslash\{0, 1, \infty\}$ and denote its Galois group by $\mathcal{G}_{\mathcal{MT}'}$. The following conjecture is well known.

Conjecture 1. *The map $\mathcal{G}_{\mathcal{MT}} \twoheadrightarrow \mathcal{G}_{\mathcal{MT}'}$ is an isomorphism.*

Some consequences of this conjecture are explained in [1, §25.5–25.7]. In particular, it implies a conjecture due to Deligne and Ihara on the outer action of $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ on the pro-ℓ fundamental group of $\mathbb{P}^1\backslash\{0, 1, \infty\}$. Another consequence is that the periods of $\mathcal{MT}(\mathbb{Z})$ are $\mathbb{Q}[\frac{1}{2\pi i}]$-linear combinations of multiple zeta values

$$\zeta(n_1, \ldots, n_r) = \sum_{0<k_1<\ldots<k_r} \frac{1}{k_1^{n_1} \ldots k_r^{n_r}}, \qquad \text{where } n_i \geq 1,\ n_r \geq 2. \tag{1.1}$$

On the other hand, M. Hoffman proposed a conjectural basis for the $\mathbb{Q}$-vector space spanned by multiple zeta values in [6]. The algebraic part of this conjecture is

Conjecture 2. *Every multiple zeta value* (1.1) *is a $\mathbb{Q}$-linear combination of*

$$\{\zeta(n_1, \ldots, n_r),\ \textit{where } n_1, \ldots, n_r \in \{2, 3\}\}. \tag{1.2}$$

In this paper we prove Conjectures 1 and 2 using motivic multiple zeta values. These are elements in a certain graded comodule $\mathcal{H}^{\mathcal{MT}_+}$ over the affine ring of functions on the prounipotent part of $\mathcal{G}_{\mathcal{MT}}$ and are graded versions of the motivic iterated integrals defined in [5]. We denote each motivic multiple zeta value by a symbol

$$\zeta^{\mathfrak{m}}(n_1, \ldots, n_r), \qquad \text{where } n_i \geq 1,\ n_r \geq 2, \tag{1.3}$$

and its period is the multiple zeta value (1.1). Note that in our setting $\zeta^{\mathfrak{m}}(2)$ is not zero, by contrast with [5]. Our main result is the following.

THEOREM 1.1. *The set of elements*

$$\{\zeta^{\mathfrak{m}}(n_1, \ldots, n_r),\ \textit{where } n_i \in \{2,3\}\} \tag{1.4}$$

are a basis of the $\mathbb{Q}$*-vector space of motivic multiple zeta values.*

Since the dimension of the basis (1.4) coincides with the known dimension for $\mathcal{H}^{\mathcal{MT}_+}$ in each degree, this implies Conjecture 1. Conjecture 2 follows from Theorem 1.1 by applying the period map. Both conjectures together imply the following

COROLLARY 1.2. *The periods of every mixed Tate motive over* $\mathbb{Z}$ *are* $\mathbb{Q}[\frac{1}{2\pi i}]$*-linear combinations of* $\zeta(n_1, \ldots, n_r)$*, where* $n_1, \ldots, n_r \in \{2,3\}$.

1.1. *Outline.* The structure of the de Rham realization of $\mathcal{G}_{\mathcal{MT}}$ is well known: there is a split exact sequence

$$1 \longrightarrow \mathcal{G}_{\mathcal{U}} \longrightarrow \mathcal{G}_{\mathcal{MT}} \longrightarrow \mathbb{G}_m \longrightarrow 1,$$

where $\mathcal{G}_{\mathcal{U}}$ is a prounipotent group whose Lie algebra is free, generated by one element σ_{2n+1} in degree $-2n-1$ for all $n \geq 1$. Let $\mathcal{A}^{\mathcal{MT}}$ be the graded affine ring of $\mathcal{G}_{\mathcal{U}}$ over $\mathbb{Q}$. It is a cofree commutative graded Hopf algebra cogenerated by one element f_{2n+1} in degree $2n+1$ for all $n \geq 1$. Consider the free comodule over $\mathcal{A}^{\mathcal{MT}}$ defined by

$$\mathcal{H}^{\mathcal{MT}_+} = \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathbb{Q}[f_2],$$

where f_2 is in degree 2, has trivial coaction, and is an artefact to keep track of even Tate twists (since multiple zeta values are real numbers, we need not consider odd Tate twists). In keeping with the usual terminology for multiple zeta values, we refer to the grading on $\mathcal{H}^{\mathcal{MT}_+}$ as the weight, which is one half the motivic weight. After making some choices, the motivic multiple zeta values (1.3) can be viewed as elements of $\mathcal{H}^{\mathcal{MT}_+}$ defined by functions on a certain subscheme of the motivic torsor of paths of $\mathbb{P}^1\backslash\{0,1,\infty\}$ from 0 to 1. They have a canonical period given by a coefficient in Drinfel′d's associator, and the element $\zeta^{\mathfrak{m}}(2)$, which is nonzero in our setting, corresponds to f_2.

Let $\mathcal{H} \subseteq \mathcal{H}^{\mathcal{MT}_+}$ denote the subspace spanned by the motivic multiple zetas. By Ihara, the action of $\mathcal{G}_{\mathcal{U}}$ on the motivic torsor of paths is determined by its action on the trivial de Rham path from 0 to 1. The dual coaction

$$\Delta : \mathcal{H} \longrightarrow \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathcal{H} \tag{1.5}$$

can be determined by a formula due to Goncharov [5].

Let $\mathcal{H}^{2,3} \subseteq \mathcal{H}$ be the vector subspace spanned by the elements (1.4). We define an increasing filtration $F_\bullet$ on $\mathcal{H}^{2,3}$, called the level, by the number of arguments n_i in $\zeta^{\mathfrak{m}}(n_1, \ldots, n_m)$ which are equal to 3. We show that $\mathcal{H}^{2,3}$ and the $F_\ell \mathcal{H}^{2,3}$ are stable under the action of $\mathcal{G}_{\mathcal{U}}$, and that $\mathcal{G}_{\mathcal{U}}$ acts trivially on the $\mathrm{gr}_\ell^F(\mathcal{H}^{2,3})$. As a consequence, the action of $\mathcal{G}_{\mathcal{U}}$ on $F_\ell \mathcal{H}^{2,3}/F_{\ell-2}\mathcal{H}^{2,3}$ factors through the abelianization $\mathcal{G}_{\mathcal{U}}^{\mathrm{ab}}$ of $\mathcal{G}_{\mathcal{U}}$. By construction, $\mathrm{gr}_\ell^F \mathcal{H}_N^{2,3}$ is spanned by elements (1.4) indexed by the words in the letters 2 and 3, with ℓ letters 3, and m letters 2, where $3\ell + 2m = N$. Let $(\mathrm{gr}_\ell^F \mathcal{H}^{2,3})^{\sim}$ be the vector space generated by the same words. The commutative Lie algebra $\mathrm{Lie}\, \mathcal{G}_{\mathcal{U}}^{\mathrm{ab}}$ is generated by one element in every degree $-2i-1$ ($i \geq 1$). We compute their actions

$$\partial_{N,\ell} : \mathrm{gr}_\ell^F \mathcal{H}_N^{2,3} \longrightarrow \bigoplus_{1<2i+1\leq N} \mathrm{gr}_{\ell-1}^F \mathcal{H}_{N-2i-1}^{2,3} \tag{1.6}$$

by constructing maps

$$\partial_{N,\ell}^{\sim} : (\mathrm{gr}_\ell^F \mathcal{H}_N^{2,3})^{\sim} \longrightarrow \bigoplus_{1<2i+1\leq N} (\mathrm{gr}_{\ell-1}^F \mathcal{H}_{N-2i-1}^{2,3})^{\sim}, \tag{1.7}$$

such that the following diagram commutes:

$$\begin{array}{ccc}
(\mathrm{gr}_\ell^F \mathcal{H}_N^{2,3})^{\sim} & \longrightarrow & \bigoplus_{1<2i+1\leq N} (\mathrm{gr}_{\ell-1}^F \mathcal{H}_{N-2i-1}^{2,3})^{\sim} \\
\downarrow & & \downarrow \\
\mathrm{gr}_\ell^F \mathcal{H}_N^{2,3} & \longrightarrow & \bigoplus_{1<2i+1\leq N} \mathrm{gr}_{\ell-1}^F \mathcal{H}_{N-2i-1}^{2,3}.
\end{array}$$

Using the explicit formula for the coaction (1.5), we write the maps $\partial_{N,\ell}^{\sim}$ as matrices $M_{N,\ell}$ whose entries are linear combinations of certain rational numbers $c_w \in \mathbb{Q}$, where w is a word in $\{2,3\}$ which has a single 3. The numbers c_w are defined as follows. We prove that for all $a, b \in \mathbb{N}$, there exist numbers $\alpha_i^{a,b} \in \mathbb{Q}$ such that

$$\zeta^{\mathfrak{m}}(\underbrace{2,\ldots,2}_{a},3,\underbrace{2,\ldots,2}_{b}) = \alpha_n^{a,b}\zeta^{\mathfrak{m}}(2n+1) + \sum_{i=1}^{n-1} \alpha_i^{a,b}\, \zeta^{\mathfrak{m}}(2i+1)\zeta^{\mathfrak{m}}(\underbrace{2,\ldots,2}_{n-i}), \tag{1.8}$$

where $n = a+b+1$. For any word w of the form $2^{\{a\}}32^{\{b\}}$, the number c_w is the coefficient $\alpha_n^{a,b}$ of $\zeta^{\mathfrak{m}}(2n+1)$ in (1.8). At this point we use a crucial arithmetic result due to Don Zagier [9], who proved an explicit formula for $\zeta(2,\ldots,2,3,2,\ldots,2)$ in terms of $\zeta(2i+1)$ and powers of π of the same shape as (1.8). Since the transcendence conjectures for multiple zeta values are not known, this does not immediately imply a formula for the coefficients $\alpha_i^{a,b}$. However, in Section 4 we show how to lift Zagier's theorem from real numbers to motivic multiple zeta values, which yields a precise formula for the coefficients $\alpha_i^{a,b}$, and in particular, c_w. From this, we deduce that the c_w satisfy certain 2-adic properties. By exploiting these properties, we show that the matrices $M_{N,\ell}$, which are rather complicated, are in fact upper-triangular to leading 2-adic order. From this, we show that the maps (1.6) are invertible for $\ell \geq 1$, and Theorem 1.1 follows by an induction on the level. The proof also shows that the level filtration is dual to the filtration induced by the descending central series of $\mathcal{G}_{\mathcal{U}}$.

P. Deligne has obtained analogous results in the case $\mathbb{P}^1\backslash\{0,\mu_N,\infty\}$, where μ_N is the set of N^{th} roots of unity, and $N=2,3,4,6$ or 8 [3]. His argument uses the depth filtration and proves that it is dual to the filtration induced by the descending central series of $\mathcal{G}_{\mathcal{U}}$. Note that in the case $N=1$ this is false, starting from weight 12.

The notes [2] might serve as an introduction to this paper.

2. **Motivic multiple zeta values**

2.1. *Preliminaries.* With the notation of [4, §5.13], let ${}_0\Pi_1$ denote the de Rham realization of the motivic torsor of paths on $\mathbb{P}^1\backslash\{0,1,\infty\}$ from 0 to 1 (with tangent vectors 1, -1 respectively). It is the functor which to any $\mathbb{Q}$-algebra R associates the set ${}_0\Pi_1(R)$ of group-like series in the algebra $R\langle\langle e_0,e_1\rangle\rangle$ of noncommutative formal power series in two generators. Its ring of affine functions over $\mathbb{Q}$ is isomorphic to

$$\mathcal{O}({}_0\Pi_1)\cong\mathbb{Q}\langle e^0,e^1\rangle, \tag{2.1}$$

which is a commutative, graded algebra equipped with the shuffle product. To every word w in the letters e^0,e^1 corresponds the function which maps a series $S\in{}_0\Pi_1(R)$ to the coefficient of w (viewed as a word in e_0,e_1) in S.

Let $\mathrm{dch}\in{}_0\Pi_1(\mathbb{R})$ denote the de Rham image of the straight line from 0 to 1 ([4, §5.16]). It is a group-like formal power series in e_0 and e_1. The coefficients of words beginning with e_1 and ending in e_0 are the multiple zeta values, and dch is also known as the Drinfel′d associator. The coefficients of e_0 and e_1 vanish, and from this, all the other coefficients are uniquely determined. Evaluation at dch is a homomorphism

$$\mathrm{dch}:\mathcal{O}({}_0\Pi_1)\longrightarrow\mathbb{R} \tag{2.2}$$

which maps a word w in e^0,e^1 to the coefficient of w in dch.

Since $\mathcal{O}({}_0\Pi_1)$ is the de Rham realization of an (ind-) mixed Tate motive over $\mathbb{Z}$, the group $\mathcal{G}_{\mathcal{MT}}$ acts upon ${}_0\Pi_1$ ([4, §5.12]). The group $\mathcal{G}_{\mathcal{MT}'}$ in the introduction is the quotient of $\mathcal{G}_{\mathcal{MT}}$ by the kernel of this action. Let $\mathcal{G}_{\mathcal{U}'}$ denote the corresponding quotient of $\mathcal{G}_{\mathcal{U}}$. We shall denote the graded ring of affine functions on $\mathcal{G}_{\mathcal{U}'}$ over $\mathbb{Q}$ by

$$\mathcal{A}=\mathcal{O}(\mathcal{G}_{\mathcal{U}'}).$$

The action $\mathcal{G}_{\mathcal{U}'}\times{}_0\Pi_1\to{}_0\Pi_1$ of the prounipotent part of $\mathcal{G}_{\mathcal{MT}'}$ gives rise to a coaction

$$\mathcal{O}({}_0\Pi_1)\longrightarrow\mathcal{A}\otimes_{\mathbb{Q}}\mathcal{O}({}_0\Pi_1). \tag{2.3}$$

Now let A denote the group of automorphisms of the de Rham fundamental groupoid of $\mathbb{P}^1\backslash\{0,1,\infty\}$ with base points $0,1$ and which respects $e_0 \in \mathrm{Lie}\,({}_0\Pi_0)$ and $e_1 \in \mathrm{Lie}\,({}_1\Pi_1)$. The action of $\mathcal{G}_{\mathcal{MT}}$ on ${}_0\Pi_1$ factors through the action of A on ${}_0\Pi_1$. The latter was computed by Y. Ihara as follows (see [4, §5.15]). Let ${}_01_1$ denote the identity element in ${}_0\Pi_1$. There is an isomorphism of schemes

$$a \mapsto a.{}_01_1 : A \xrightarrow{\sim} {}_0\Pi_1. \tag{2.4}$$

Via this identification, the action of A on ${}_0\Pi_1$ can be computed explicitly. The morphism (2.4) induces a linear morphism from the Lie algebra of A to the Lie algebra of ${}_0\Pi_1$. It transforms the Lie bracket of $\mathrm{Lie}(A)$ into Ihara's bracket. The dual coaction

$$\mathcal{O}({}_0\Pi_1) \xrightarrow{\Delta} \mathcal{O}(A) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1) \cong \mathcal{O}({}_0\Pi_1) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1) \tag{2.5}$$

was computed by Goncharov in [5, Th. 1.2], except that the two right-hand factors are interchanged. The formula involves $\mathcal{O}({}_a\Pi_b)$ for all $a,b \in \{0,1\}$, but it can easily be rewritten in terms of $\mathcal{O}({}_0\Pi_1)$ only. (This is the content of Properties I0, I1, I3 below.) It follows that the coaction (2.3) is obtained by composing Δ of (2.5) with the map

$$\begin{aligned} \mathcal{O}({}_0\Pi_1) &\longrightarrow \mathcal{A} \\ \phi &\mapsto\ g \mapsto \phi(g.{}_01_1) \end{aligned} \tag{2.6}$$

applied to the left-hand factor of $\mathcal{O}({}_0\Pi_1) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1)$. Note that since $\mathbb{G}_m$ acts trivially on ${}_01_1$, the map (2.6) necessarily loses information about the weight grading.

2.2. *Definition of motivic* MZV*s*. Let $I \subset \mathcal{O}({}_0\Pi_1)$ be the kernel of the map dch (2.2). It describes the $\mathbb{Q}$-linear relations between multiple zeta values. Let $J^{\mathcal{MT}} \subseteq I$ be the largest graded ideal contained in I which is stable under the coaction (2.3).

Definition 2.1. Define the graded coalgebra of motivic multiple zeta values to be

$$\mathcal{H} = \mathcal{O}({}_0\Pi_1)/J^{\mathcal{MT}}. \tag{2.7}$$

A word w in the letters 0 and 1 defines an element in (2.1). Denote its image in $\mathcal{H}$ by

$$I^{\mathfrak{m}}(0;w;1) \in \mathcal{H}, \tag{2.8}$$

which we shall call a motivic iterated integral. For $n_0 \geq 0$ and $n_1,\ldots,n_r \geq 1$, let

$$\zeta^{\mathfrak{m}}_{n_0}(n_1,\ldots,n_r) = I^{\mathfrak{m}}(0;\underbrace{0,\ldots,0}_{n_0},\underbrace{1,0,\ldots,0}_{n_1},\ldots,\underbrace{1,0,\ldots,0}_{n_r};1). \tag{2.9}$$

In the case when $n_0 = 0$, we shall simply write this $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$ and call it a motivic multiple zeta value. As usual, we denote the grading on $\mathcal{H}$ by a subscript.

The coaction (2.3) induces a coaction $\Delta : \mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$. By the discussion at the end of Section 2.1, it can be computed from (2.5); i.e., the following diagram commutes:

$$\begin{array}{ccc} \mathcal{O}({}_0\Pi_1) & \longrightarrow & \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1) \\ \downarrow & & \downarrow \\ \mathcal{H} & \longrightarrow & \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}. \end{array} \tag{2.10}$$

Furthermore, the map dch (2.2) factors through $\mathcal{H}$. The resulting homomorphism from $\mathcal{H}$ to $\mathbb{R}$ shall be called the period map, which we denote by

$$\mathrm{per} : \mathcal{H} \longrightarrow \mathbb{R}. \tag{2.11}$$

Remark 2.2. The ideal $J^{\mathcal{MT}}$ could be called the ideal of motivic relations. A homogeneous linear combination $R \subset \mathcal{O}({}_0\Pi_1)$ of words is a relation between motivic multiple zetas if

1) R holds numerically (i.e., $\mathrm{per}(R) = 0$),
2) R' holds numerically for all transforms R' of R under the coaction (2.3).

This argument is used in Section 4 to lift certain relations from multiple zetas to their motivic versions, and can be made into a kind of numerical algorithm (see [2]).

2.3. *The role of* $\zeta^{\mathfrak{m}}(2)$. It is also convenient to consider the dual point of view. Let $\mathcal{Y} = \operatorname{Spec} \mathcal{H}$. It is the Zariski closure of the $\mathcal{G}_{\mathcal{MT}}$-orbit of dch, i.e.,

$$\mathcal{Y} = \overline{\mathcal{G}_{\mathcal{MT}}.\mathrm{dch}}.$$

Thus $\mathcal{Y}$ is a subscheme of the extension of scalars ${}_0\Pi_1 \otimes_{\mathbb{Q}} \mathbb{R}$, but is in fact defined over $\mathbb{Q}$ since dch is Betti-rational. Let τ denote the action of $\mathbb{G}_m$ on ${}_0\Pi_1$. The map $\tau(\lambda)$ multiplies elements of degree d by λ^d. Let us choose a rational point $\gamma \in \mathcal{Y}(\mathbb{Q})$ which is even, i.e., $\tau(-1)\gamma = \gamma$ (see [4, §5.20]). Since $\mathcal{G}_{\mathcal{U}'}$ is the quotient of $\mathcal{G}_{\mathcal{U}}$ through which it acts on $\mathcal{Y}$, we obtain an isomorphism

$$\begin{array}{c} \mathcal{G}_{\mathcal{U}'} \times \mathbb{A}^1 \overset{\sim}{\longrightarrow} \mathcal{Y} \\ (g, t) \mapsto g\,\tau(\sqrt{t}).\gamma. \end{array} \tag{2.12}$$

The parameter t is retrieved by taking the coefficient of $e_0 e_1$ in the series $g\,\tau(\sqrt{t}).\gamma$. Thus (2.12) gives rise to an isomorphism of graded algebra comodules

$$\mathcal{H} \cong \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)], \tag{2.13}$$

which depends on γ, where $\Delta(\zeta^{\mathfrak{m}}(2)) = 1 \otimes \zeta^{\mathfrak{m}}(2)$ (Lemma 3.2). Most of our constructions will not in fact depend on this choice of γ, but we may fix it once and for all. Since the leading term of dch is ${}_0 1_1$, we have $\lim_{t\to 0} \tau(t)\mathrm{dch} = {}_0 1_1$, which shows that

$$\mathcal{G}_{\mathcal{U}'} . {}_0 1_1 \subseteq \mathcal{Y}.$$

Thus the map $\mathcal{H} \to \mathcal{A}$ is induced by (2.6) and sends $\zeta^{\mathfrak{m}}(2)$ to zero.

Definition 2.3. Let us denote the graded ring of affine functions on $\mathcal{G}_{\mathcal{U}}$ over $\mathbb{Q}$ by

$$\mathcal{A}^{\mathcal{MT}} = \mathcal{O}(\mathcal{G}_{\mathcal{U}})$$

and define $\mathcal{H}^{\mathcal{MT}_+} = \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathbb{Q}[f_2]$, where the elements f_2^k are in degree $2k$. Thus $\mathcal{H}^{\mathcal{MT}_+}$ is a graded algebra comodule over $\mathcal{A}^{\mathcal{MT}}$, and its grading shall be called the weight hereafter. We shall also denote the coaction by

$$\Delta : \mathcal{H}^{\mathcal{MT}_+} \longrightarrow \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathcal{H}^{\mathcal{MT}_+}. \tag{2.14}$$

It is uniquely determined by the property $\Delta f_2 = 1 \otimes f_2$.

In conclusion, the inclusion $\mathcal{A} \to \mathcal{A}^{\mathcal{MT}}$ which is dual to the quotient map $\mathcal{G}_{\mathcal{U}} \to \mathcal{G}_{\mathcal{U}'}$ induces an injective morphism of graded algebra comodules

$$\mathcal{H} \longrightarrow \mathcal{H}^{\mathcal{MT}_+} \tag{2.15}$$

which sends $\zeta^{\mathfrak{m}}(2)$ to f_2, by (2.13). The map (2.15) implicitly depends on the choice of γ. Abusively, we sometimes identify motivic multiple zeta values with their images under (2.15), i.e., as elements in $\mathcal{H}^{\mathcal{MT}_+}$.

2.4. *Main properties.* In order to write down the formula for the coaction on the motivic iterated integrals, we must slightly extend the notation (2.8). For all sequences $a_0, \ldots, a_{n+1} \in \{0,1\}$, we define elements

$$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) \in \mathcal{H}_n \tag{2.16}$$

which are given by (2.8) if $a_0 = 0$ and $a_{n+1} = 1$, and are uniquely extended to all sets of indices $a_i \in \{0,1\}$ as follows. For any $a, b \in \{0,1\}$, write

$$I_{a,b} = \sum_{n \geq 0, a_i \in \{0,1\}} I^{\mathfrak{m}}(a; a_1, \ldots, a_n; b) e_{a_1} \ldots e_{a_n}$$

and demand that $I_{a,b} = 1$ if $a = b$, and $I_{a,b} = I_{b,a}^{-1}$.

We summarize the properties satisfied by (2.16) for later reference.

- I0: If $n \geq 1$, then $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) = 0$ if $a_0 = a_{n+1}$ or $a_1 = \cdots = a_n$.
- I1: $I^{\mathfrak{m}}(a_0; a_1) = 1$ for all $a_0, a_1 \in \{0,1\}$ and $\zeta^{\mathfrak{m}}(2) = f_2$.
- I2: *Shuffle product* (*special case*). For $k \geq 0, n_1, \ldots, n_r \geq 1$, we have

$$\zeta_k^{\mathfrak{m}}(n_1, \ldots, n_r) = (-1)^k \sum_{i_1 + \ldots + i_r = k} \binom{n_1 + i_1 - 1}{i_1} \ldots \binom{n_r + i_r - 1}{i_r} \zeta^{\mathfrak{m}}(n_1 + i_1, \ldots, n_r + i_r).$$

I3: *Reflection formulae.* For all $a_1, \dots, a_n \in \{0,1\}$,

$$I^{\mathfrak{m}}(0; a_1, \dots, a_n; 1) = (-1)^n I^{\mathfrak{m}}(1; a_n, \dots, a_1; 0) = I^{\mathfrak{m}}(0; 1-a_n, \dots, 1-a_1; 1).$$

The motivic multiple zeta values of [5] are, up to a possible sign, the images of (2.16) under the map $\pi : \mathcal{H} \to \mathcal{A}$ which sends $\zeta^{\mathfrak{m}}(2)$ to zero. We have shown (see (2.5), (2.10))

Theorem 2.4. *The coaction for the motivic multiple zeta values*

$$\Delta : \mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H} \tag{2.17}$$

is given by the same formula as [5, Th. 1.2], *with the factors interchanged. In particular, if* $a_0, \dots, a_{n+1} \in \{0,1\}$, *then* $\Delta\, I^{\mathfrak{m}}(a_0; a_1, \dots, a_n; a_{n+1})$ *equals*

$$\sum_{\substack{i_0 < i_1 < \dots < i_{k+1} \\ i_0 = 0, i_{k+1} = n+1}} \pi\Big(\prod_{p=0}^{k} I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, .\,.\,, a_{i_{p+1}-1}; a_{i_{p+1}})\Big) \otimes I^{\mathfrak{m}}(a_0; a_{i_1}, .\,.\,, a_{i_k}; a_{n+1}), \tag{2.18}$$

where the first sum is also over all values of k *for* $0 \le k \le n$.

Lastly, the period map $\mathrm{per} : \mathcal{H} \to \mathbb{R}$ can be computed as follows:

$$per\Big(I^{\mathfrak{m}}(a_0; a_1, \dots, a_n; a_{n+1})\Big) = \int_{a_0}^{a_{n+1}} \omega_{a_1} \dots \omega_{a_n},$$

where $\omega_0 = \frac{dt}{t}, \omega_1 = \frac{dt}{1-t}$, and the right-hand side is a shuffle-regularized iterated integral (e.g., [4] §5.16). Note that the sign of ω_1 varies in the literature. Here, the signs are chosen such that the period of the motivic multiple zeta values are

$$\mathrm{per}\big(\zeta^{\mathfrak{m}}(n_1, \dots, n_r)\big) = \zeta(n_1, \dots, n_r) \quad \text{when } n_r \ge 2. \tag{2.19}$$

2.5. *Structure of* $\mathcal{H}^{\mathcal{MT}_+}$. The structure of $\mathcal{MT}(\mathbb{Z})$ is determined by the data

$$\mathrm{Ext}^1_{\mathcal{MT}(\mathbb{Z})}(\mathbb{Q}(0), \mathbb{Q}(n)) \cong \begin{cases} \mathbb{Q} & \text{if } n \ge 3 \text{ is odd,} \\ 0 & \text{otherwise} \end{cases}$$

and the fact that the Ext^2's vanish. Thus $\mathcal{MT}(\mathbb{Z})$ is equivalent to the category of representations of a group scheme $\mathcal{G}_{\mathcal{MT}}$ over $\mathbb{Q}$, which is a semi-direct product

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

where $\mathcal{G}_{\mathcal{U}}$ is a prounipotent group whose Lie algebra $\mathrm{Lie}\, \mathcal{G}_{\mathcal{U}}$ is isomorphic to the free Lie algebra with one generator σ_{2i+1} in every degree $-2i-1$ for $i \ge 1$. Let $\mathcal{A}^{\mathcal{MT}}$ be the graded ring of functions on $\mathcal{G}_{\mathcal{U}}$, where the grading is with respect to the action of $\mathbb{G}_m$. Since the degrees of the σ_{2i+1} tend to minus infinity, no information is lost in passing to the graded version $(\mathrm{Lie}\, \mathcal{G}_{\mathcal{U}})^{\mathrm{gr}}$ of $\mathrm{Lie}\, \mathcal{G}_{\mathcal{U}}$ (Proposition 2.2 (ii) of [4]). By the above, $\mathcal{A}^{\mathcal{MT}}$ is noncanonically isomorphic to the graded dual of the universal envelopping algebra of $(\mathrm{Lie}\,\mathcal{G}_{\mathcal{U}})^{\mathrm{gr}}$ over $\mathbb{Q}$. We shall denote this by

$$\mathcal{U}' = \mathbb{Q}\langle f_3, f_5, \ldots \rangle.$$

Its underlying vector space has a basis consisting of noncommutative words in symbols f_{2i+1} in degree $2i+1$, and the multiplication is given by the shuffle product ш. The coproduct is given by the following deconcatenation formula:

$$\Delta : \mathcal{U}' \to \mathcal{U}' \otimes_{\mathbb{Q}} \mathcal{U}' \tag{2.20}$$

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

when $n \geq 0$. Let us consider the following universal comodule:

$$\mathcal{U} = \mathbb{Q}\langle f_3, f_5, \ldots \rangle \otimes_{\mathbb{Q}} \mathbb{Q}[f_2], \tag{2.21}$$

where f_2 is of degree 2, commutes with all generators f_{2n+1} of odd degree, and the coaction $\Delta : \mathcal{U} \to \mathcal{U}' \otimes_{\mathbb{Q}} \mathcal{U}$ satisfies $\Delta(f_2) = 1 \otimes f_2$. The degree will also be referred to as the weight. By the above discussion, there exists a noncanonical isomorphism

$$\phi : \mathcal{H}^{\mathcal{MT}_+} \cong \mathcal{U} \tag{2.22}$$

of algebra comodules which sends f_2 to f_2. These notations are useful for explicit computations, for which it can be convenient to vary the choice of map ϕ (see [2]).

LEMMA 2.5. *Let* $d_k = \dim \mathcal{U}_k$, *where* $\mathcal{U}_k$ *is the graded piece of* $\mathcal{U}$ *of weight* k. *Then*

$$\sum_{k \geq 0} d_k t^k = \frac{1}{1 - t^2 - t^3}. \tag{2.23}$$

In particular, $d_0 = 1, d_1 = 0,\ d_2 = 1,$ *and* $d_k = d_{k-2} + d_{k-3}$ *for* $k \geq 3$.

Proof. The Poincaré series of $\mathbb{Q}\langle f_3, f_5, \ldots \rangle$ is given by $\frac{1}{1-t^3-t^5-\ldots} = \frac{1-t^2}{1-t^2-t^3}$. If we multiply by the Poincaré series $\frac{1}{1-t^2}$ for $\mathbb{Q}[f_2]$, we obtain (2.23). ☐

Definition 2.6. It will be convenient to define an element $f_{2n} \in \mathcal{U}_{2n}$, for $n \geq 2$, by

$$f_{2n} = b_n f_2^n,$$

where $b_n \in \mathbb{Q}^\times$ is the constant in Euler's relation $\zeta(2n) = b_n \zeta(2)^n$.

Let us denote the Lie coalgebra of indecomposable elements of $\mathcal{U}'$ by

$$L = \frac{\mathcal{U}'_{>0}}{\mathcal{U}'_{>0}\mathcal{U}'_{>0}}, \tag{2.24}$$

and for any $N \geq 1$, let $\pi_N : \mathcal{U}'_{>0} \to L_N$ denote the quotient map followed by projection onto the graded part of weight N. For any $r \geq 1$, consider the map

$$D_{2r+1} : \mathcal{U} \longrightarrow L_{2r+1} \otimes_{\mathbb{Q}} \mathcal{U} \tag{2.25}$$

defined by composing $\Delta' = \Delta - 1 \otimes \mathrm{id}$ with $\pi_{2r+1} \otimes \mathrm{id}$. Let

$$D_{<N} = \bigoplus_{1<2i+1<N} D_{2i+1}. \tag{2.26}$$

Lemma 2.7. $(\ker D_{<N}) \cap \mathcal{U}_N = \mathbb{Q}\, f_N$.

Proof. Every element $\xi \in \mathcal{U}_N$ can be uniquely written in the form

$$\xi = \sum_{1<2r+1<N} f_{2r+1} v_r + c f_N,$$

where $c \in \mathbb{Q}$, $v_r \in \mathcal{U}_{N-2r-1}$, and the multiplication on the right-hand side is the concatenation product. The graded dual of L is isomorphic to the free Lie algebra with generators $f^\vee_{2r+1}$ in degrees $-2r-1$ dual to the f_{2r+1}. Each element $f^\vee_{2r+1}$ defines a map $f^\vee_{2r+1} : L \to \mathbb{Q}$ which sends f_{2r+1} to 1. By definition,

$$(f^\vee_{2r+1} \otimes \mathrm{id}) \circ D_{2r+1}\xi = v_r$$

for all $1 < 2r+1 < N$. It follows immediately that if ξ is in the kernel of $D_{<N}$, then it is of the form $\xi = c f_N$. Since $D_{<N} f_N = 0$, the result follows. $\square$

3. Cogenerators of the coalgebra

3.1. *Infinitesimal coaction.* In order to simplify the formula (2.18), let

$$\mathcal{L} = \frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0}\mathcal{A}_{>0}} \tag{3.1}$$

denote the Lie coalgebra of $\mathcal{A} = \mathcal{H}/\zeta^{\mathfrak{m}}(2)\mathcal{H}$, and let $\pi : \mathcal{H}_{>0} \to \mathcal{L}$ denote the quotient map. Since $\mathcal{L}$ inherits a weight grading from $\mathcal{H}$, let $\mathcal{L}_N$ denote the elements of $\mathcal{L}$ of homogeneous weight N, and let $p_N : \mathcal{L} \to \mathcal{L}_N$ be the projection map.

Definition 3.1. By analogy with (2.25) and (2.26), for every $r \geq 1$, define a map

$$D_{2r+1} : \mathcal{H} \longrightarrow \mathcal{L}_{2r+1} \otimes_{\mathbb{Q}} \mathcal{H}$$

to be $(\pi \otimes \mathrm{id}) \circ \Delta'$, where $\Delta' = \Delta - 1 \otimes \mathrm{id}$, followed by $p_{2r+1} \otimes \mathrm{id}$. Let

$$D_{<N} = \bigoplus_{3\leq 2r+1<N} D_{2r+1}. \tag{3.2}$$

It follows from this definition that the maps D_n, where $n = 2r+1$, are derivations:

$$D_n(\xi_1\xi_2) = (1 \otimes \xi_1)D_n(\xi_2) + (1 \otimes \xi_2)D_n(\xi_1) \quad \text{for all } \xi_1, \xi_2 \in \mathcal{H}. \tag{3.3}$$

By (2.18), the action of D_n on $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_N; a_{N+1})$ is given by

$$\sum_{p=0}^{N-n} \pi\big(I^{\mathfrak{m}}(a_p; a_{p+1}, \ldots, a_{p+n}; a_{p+n+1})\big) \otimes I^{\mathfrak{m}}(a_0; a_1, \ldots, a_p, a_{p+n+1}, \ldots, a_N; a_{N+1}). \tag{3.4}$$

By analogy with the Connes-Kreimer coproduct, we call the sequence of consecutive elements $(a_p; a_{p+1}, \ldots, a_{p+n}; a_{p+n+1})$ on the left a *subsequence of length* n of the original sequence and $(a_0; a_1, \ldots, a_p, a_{p+n+1}, \ldots, a_N; a_{N+1})$ will be called the *quotient sequence*.

3.2. *Zeta elements and kernel of* $D_{<N}$.

LEMMA 3.2. *Let* $n \geq 1$. *The zeta element* $\zeta^{\mathfrak{m}}(2n+1) \in \mathcal{H}$ *is nonzero and satisfies*

$$\Delta\, \zeta^{\mathfrak{m}}(2n+1) = 1 \otimes \zeta^{\mathfrak{m}}(2n+1) + \pi(\zeta^{\mathfrak{m}}(2n+1)) \otimes 1.$$

Furthermore, Euler's relation $\zeta(2n) = b_n \zeta(2)^n$, *where* $b_n \in \mathbb{Q}$, *holds for the* $\zeta^{\mathfrak{m}}$*'s:*

$$\zeta^{\mathfrak{m}}(2n) = b_n \zeta^{\mathfrak{m}}(2)^n. \tag{3.5}$$

Proof. Consider $\zeta^{\mathfrak{m}}(N) = I^{\mathfrak{m}}(0; 10^{N-1}; 1)$, where 10^{N-1} denotes a 1 followed by $N-1$ zeros. By relation I0, its strict subsequences of length at least one are killed by $I^{\mathfrak{m}}$, and so $\Delta\, \zeta^{\mathfrak{m}}(N) = 1 \otimes \zeta^{\mathfrak{m}}(N) + \pi(\zeta^{\mathfrak{m}}(N)) \otimes 1$ by (3.4). From the structure of $\mathcal{U}$, it follows that an isomorphism ϕ (2.22) maps $\zeta^{\mathfrak{m}}(2n+1)$ to $\alpha_n f_{2n+1}$ for some $\alpha_n \in \mathbb{Q}$ and $\zeta^{\mathfrak{m}}(2n)$ to $\beta_n f_2^n$ for some $\beta_n \in \mathbb{Q}$. Taking the period map yields $\alpha_n \neq 0$, and $\beta_n = \zeta(2n)\zeta(2)^{-n} = b_n$. $\square$

We can therefore normalize our choice of isomorphism (2.22) so that

$$\mathcal{H} \subseteq \mathcal{H}^{\mathcal{MT}_+} \xrightarrow{\phi} \mathcal{U}$$

maps $\zeta^{\mathfrak{m}}(2n+1)$ to f_{2n+1}. By Definition 2.6, we can therefore write

$$\phi(\zeta^{\mathfrak{m}}(N)) = f_N \quad \text{for all} \quad N \geq 2. \tag{3.6}$$

In particular, $\zeta^{\mathfrak{m}}(2)$ and $\zeta^{\mathfrak{m}}(2n+1)$, for $n \geq 1$, are algebraically independent in $\mathcal{H}$.

THEOREM 3.3. *Let* $N \geq 2$. *The kernel of* $D_{<N}$ *is one-dimensional in weight* N:

$$\ker D_{<N} \cap \mathcal{H}_N = \mathbb{Q}\, \zeta^{\mathfrak{m}}(N).$$

Proof. This follows from Lemma 2.7, via such an isomorphism ϕ. $\square$

Note that the map $\mathcal{L} \to L$ of Lie coalgebras induced by the inclusion $\mathcal{A} \subseteq \mathcal{A}^{\mathcal{MT}} \cong \mathcal{U}'$ is also injective, by standard results on Hopf algebras.

3.3. *Some relations between motivic multiple zeta values.* Using Theorem 3.3 we lift relations between multiple zeta values to their motivic versions. Hereafter let $2^{\{n\}}$ denote a sequence of n consecutive 2's, and let $\zeta^{\mathfrak{m}}(2^{\{0\}}) = 1 \in \mathcal{H}$. For any word w in the alphabet $\{2,3\}$, define the weight of w to be $2\deg_2 w + 3\deg_3 w$.

LEMMA 3.4. *The element $\zeta^{\mathfrak{m}}(2^{\{n\}})$ is a rational multiple of $\zeta^{\mathfrak{m}}(2)^n$.*

Proof. For reasons of parity, every strict subsequence of $(0;1010\ldots10;1)$ of odd length begins and ends in the same symbol, and corresponds to a zero motivic iterated integral by I0. Therefore $D_{2r+1}\zeta^{\mathfrak{m}}(2^{\{n\}}) = 0$ for all $r \geq 1$. By Proposition 3.3, it is a multiple of $\zeta^{\mathfrak{m}}(2n)$, that is $\zeta^{\mathfrak{m}}(2)^n$. The multiple is equal to $\zeta(2^{\{n\}})/\zeta(2)^n > 0$. □

The coefficient in the lemma can be determined by the well-known formula

$$\zeta(2^{\{n\}}) = \frac{\pi^{2n}}{(2n+1)!}. \tag{3.7}$$

We need the following trivial observation, valid for $n \geq 1$:

$$\zeta_1^{\mathfrak{m}}(2^{\{n\}}) = -2\sum_{i=0}^{n-1} \zeta^{\mathfrak{m}}(2^{\{i\}}32^{\{n-1-i\}}), \tag{3.8}$$

which follows immediately from relation I2.

LEMMA 3.5. *Let $a,b \geq 0$ and $1 \leq r \leq a+b$. Then*

$$D_{2r+1}\,\zeta^{\mathfrak{m}}(2^{\{a\}}32^{\{b\}}) = \pi(\xi^r_{a,b}) \otimes \zeta^{\mathfrak{m}}(2^{\{a+b+1-r\}}),$$

where $\xi^r_{a,b}$ is given by (sum over all indices $\alpha,\beta \geq 0$ satisfying $\alpha+\beta+1 = r$)

$$\xi^r_{a,b} = \sum_{\substack{\alpha\leq a\\ \beta\leq b}} \zeta^{\mathfrak{m}}(2^{\{\alpha\}}32^{\{\beta\}}) - \sum_{\substack{\alpha\leq a\\ \beta< b}} \zeta^{\mathfrak{m}}(2^{\{\beta\}}32^{\{\alpha\}}) + \big(\mathbb{I}(b\geq r) - \mathbb{I}(a \geq r)\big)\,\zeta_1^{\mathfrak{m}}(2^{\{r\}}).$$

The symbol $\mathbb{I}$ denotes the indicator function.

Proof. The element $\zeta^{\mathfrak{m}}(w)$, where $w = 2^{\{a\}}32^{\{b\}}$, is represented by the sequence

$$I^{\mathfrak{m}}(0;10\ldots1\mathbf{00}10\ldots10;1).$$

By parity, every subsequence of length $2r+1$ which does not straddle the subsequence **00** begins and ends in the same symbol. Its motivic iterated integral vanishes by I0, so it does not contribute to D_{2r+1}. The remaining subsequences are of the form

$$I^{\mathfrak{m}}(0;\underbrace{10\ldots10}_{\alpha}1\mathbf{00}\underbrace{10\ldots10}_{\beta};1) = \zeta^{\mathfrak{m}}(2^{\{\alpha\}}32^{\{\beta\}}),$$

where $\alpha \leq a$, $\beta \leq b$, and $\alpha + \beta + 1 = r$, which gives rise to the first sum, or

$$I^{\mathfrak{m}}(1; \underbrace{01\ldots01}_{\alpha}\,\mathbf{00}1\,\underbrace{01\ldots01}_{\beta}; 0) = -\zeta^{\mathfrak{m}}(2^{\{\beta\}}32^{\{\alpha\}}),$$

which gives the second sum by I3. In this case $\beta < b$. Finally, we can also have

$$I^{\mathfrak{m}}(1; \underbrace{01\ldots01}_{r}\,\mathbf{0}; \mathbf{0}) = -\zeta^{\mathfrak{m}}_1(2^{\{r\}}), \text{ or } I^{\mathfrak{m}}(\mathbf{0}; \mathbf{0}\,\underbrace{10\ldots10}_{r}; 1) = \zeta^{\mathfrak{m}}_1(2^{\{r\}}),$$

which gives rise to the last two terms. The quotient sequences are the same in all cases, and equal to $I^{\mathfrak{m}}(0; 10\ldots10; 1)$. This proves the formula. $\square$

The following trivial observation follows from Lemma 3.2:

$$D_{2r+1}\zeta^{\mathfrak{m}}(N) = \pi(\zeta^{\mathfrak{m}}(2r+1)) \otimes \delta_{N,2r+1}, \qquad N \geq 2, r \geq 1, \tag{3.9}$$

where $\delta_{i,j}$ denotes the Kronecker delta.

Corollary 3.6. *Let w be a word in $\{2,3\}^{\times}$ of weight $2n+1$ which has many 2's and a single 3. Then there exist unique numbers $\alpha_i \in \mathbb{Q}$ such that*

$$\zeta^{\mathfrak{m}}(w) = \sum_{i=1}^{n} \alpha_i\, \zeta^{\mathfrak{m}}(2i+1)\, \zeta^{\mathfrak{m}}(2^{\{n-i\}}). \tag{3.10}$$

Proof. By induction on the weight of w. Suppose the result is true for $1 \leq n < N$. Then for a word $w = 2^{\{a\}}32^{\{b\}}$ of weight $2N+1$, the elements $\xi^r_{a,b}$ of the previous lemma, for $1 \leq r < N$, are of the form (3.10). In particular, there exists some rational number α_r such that $\xi^r_{a,b} \equiv \alpha_r\, \zeta^{\mathfrak{m}}(2r+1)$ modulo products. It follows that for $1 \leq r < N$,

$$D_{2r+1}\, \zeta^{\mathfrak{m}}(w) = \alpha_r \pi(\zeta^{\mathfrak{m}}(2r+1)) \otimes \zeta^{\mathfrak{m}}(2^{\{N-r\}})$$

and so the left and right-hand sides of (3.10) have the same image under $D_{<2N+1}$ by (3.3) and (3.9). By Theorem 3.3, they differ by a rational multiple of $\zeta^{\mathfrak{m}}(2N+1)$. $\square$

The previous corollary leads us to the following definition.

Definition 3.7. Let w be a word in $\{2,3\}^{\times}$ of weight $2n+1$ with a single 3. Define the *coefficient* $c_w \in \mathbb{Q}$ of $\zeta^{\mathfrak{m}}(w)$ to be the coefficient of $\zeta^{\mathfrak{m}}(2n+1)$ in equation (3.10). By (3.8), we can define the coefficient c_{12^n} of $\zeta^{\mathfrak{m}}_1(2^{\{n\}})$ in the same way. It satisfies

$$c_{12^n} = -2 \sum_{i=0}^{n-1} c_{2^i 3 2^{n-i-1}}. \tag{3.11}$$

Thus for any $w \in \{2,3\}^{\times}$ of weight $2n+1$ which contains a single 3, we have

$$\pi(\zeta^{\mathfrak{m}}(w)) = c_w \pi(\zeta^{\mathfrak{m}}(2n+1)). \tag{3.12}$$

Later on, we shall work not only with the actual coefficients $c_w \in \mathbb{Q}$, whose properties are described in the following section, but also with formal versions C_w of these coefficients (later to be specialized to c_w) purely to simplify calculations.

LEMMA 3.8. *For all $n \geq 1$, the coefficient c_{12^n} is equal to $2(-1)^n$. We have*

$$\zeta_1^{\mathfrak{m}}(2^{\{n\}}) = 2\sum_{i=1}^{n}(-1)^i\zeta^{\mathfrak{m}}(2i+1)\zeta^{\mathfrak{m}}(2^{\{n-i\}}).$$

Proof. Granting the motivic stuffle product formula [7], [8] for our version of motivic multiple zeta values in which $\zeta^{\mathfrak{m}}(2)$ is nonzero, we have

$$\begin{aligned}
\zeta^{\mathfrak{m}}(3)\zeta^{\mathfrak{m}}(2^{\{n-1\}}) &= \sum_{i=0}^{n-1}\zeta^{\mathfrak{m}}(2^{\{i\}}32^{\{n-1-i\}}) + \sum_{i=0}^{n-2}\zeta^{\mathfrak{m}}(2^{\{i\}}52^{\{n-2-i\}}),\\
\zeta^{\mathfrak{m}}(5)\zeta^{\mathfrak{m}}(2^{\{n-2\}}) &= \sum_{i=0}^{n-2}\zeta^{\mathfrak{m}}(2^{\{i\}}52^{\{n-2-i\}}) + \sum_{i=0}^{n-3}\zeta^{\mathfrak{m}}(2^{\{i\}}72^{\{n-3-i\}}),\\
\vdots \qquad &\quad\ \vdots \qquad\qquad\qquad\qquad \vdots\\
\zeta^{\mathfrak{m}}(2n-1)\zeta^{\mathfrak{m}}(2) &= \zeta^{\mathfrak{m}}(2n-1,2) + \zeta^{\mathfrak{m}}(2,2n-1) + \zeta^{\mathfrak{m}}(2n+1).
\end{aligned}$$

Taking the alternating sum of each row gives the equation

$$\sum_{i=0}^{n-1}\zeta^{\mathfrak{m}}(2^{\{i\}}32^{\{n-1-i\}}) = -2\sum_{i=1}^{n}(-1)^i\zeta^{\mathfrak{m}}(2i+1)\zeta^{\mathfrak{m}}(2^{\{n-i\}}).$$

This implies the lemma by (3.8). Alternatively, we can use the general method for lifting relations from real multiple zeta values to their motivic versions given in [2]. For this, it only suffices to consider the above relations modulo products and modulo $\zeta^{\mathfrak{m}}(2)$ to obtain the coefficients of $\zeta^{\mathfrak{m}}(2n+1)$, which leads to the same result. $\square$

4. Arithmetic of the coefficients c_w

The key arithmetic input is an evaluation of certain multiple zeta values which is due to Don Zagier. Using the operators $D_{<N}$ we shall lift this result to motivic multiple zetas. First, let us define for any $a, b, r \in \mathbb{N}$,

$$A^r_{a,b} = \binom{2r}{2a+2} \quad\text{and}\quad B^r_{a,b} = \left(1-2^{-2r}\right)\binom{2r}{2b+1}.$$

Note that $A^r_{a,b}$ (respectively $B^r_{a,b}$) only depends on r, a (resp. r, b).

THEOREM 4.1 (Don Zagier [9]). *Let $a, b \geq 0$. Then*

$$\zeta(2^{\{a\}}32^{\{b\}}) = 2\sum_{r=1}^{a+b+1}(-1)^r(A^r_{a,b} - B^r_{a,b})\,\zeta(2r+1)\,\zeta(2^{\{a+b+1-r\}}).$$

4.1. *Motivic version.* To prove that the arithmetic formula lifts to the level of motivic multiple zeta values requires showing that it is compatible with the coaction (2.17). This is equivalent to the following compatibility condition between the coefficients.

LEMMA 4.2. *For any $a, b \geq 0$, and $1 \leq r \leq a+b+1$, we have*

$$\sum_{\substack{\alpha\leq a\\ \beta\leq b}} A^r_{\alpha,\beta} - \sum_{\substack{\alpha\leq a\\ \beta< b}} A^r_{\beta,\alpha} + \mathbb{I}(b\geq r) - \mathbb{I}(a\geq r) = A^r_{a,b},$$

$$\sum_{\substack{\alpha\leq a\\ \beta\leq b}} B^r_{\alpha,\beta} - \sum_{\substack{\alpha\leq a\\ \beta< b}} B^r_{\beta,\alpha} = B^r_{a,b},$$

where all sums are over sets of indices $\alpha, \beta \geq 0$ satisfying $\alpha+\beta+1 = r$.

Proof. Exercise, using $A^{\alpha+\beta+1}_{\alpha,\beta} = A^{\alpha+\beta+1}_{\beta-1,\alpha+1}$ and $B^{\alpha+\beta+1}_{\alpha,\beta} = B^{\alpha+\beta+1}_{\beta,\alpha}$. □

We now show that Zagier's theorem lifts to motivic multiple zetas.

THEOREM 4.3. *Let $a, b \geq 0$. Then*

$$\zeta^{\mathfrak{m}}(2^{\{a\}}32^{\{b\}}) = 2\sum_{r=1}^{a+b+1} (-1)^r (A^r_{a,b} - B^r_{a,b})\, \zeta^{\mathfrak{m}}(2r+1)\, \zeta^{\mathfrak{m}}(2^{\{a+b+1-r\}})\ . \tag{4.1}$$

In particular, if $w = 2^{\{a\}}32^{\{b\}}$, then the coefficient c_w is given by

$$c_w = 2\,(-1)^{a+b+1}\Big(A^{a+b+1}_{a,b} - B^{a+b+1}_{a,b}\Big)\ . \tag{4.2}$$

Proof. The proof is by induction on the weight. Suppose that (4.1) holds for all $a+b<N$ and let $a, b \geq 0$ such that $a+b=N$. Then by Lemma 3.5,

$$D_{2r+1}\, \zeta^{\mathfrak{m}}(2^{\{a\}}32^{\{b\}}) = \pi(\xi^r_{a,b}) \otimes \zeta^{\mathfrak{m}}(2^{\{a+b+1-r\}})$$

for $1 \leq r \leq N$. The second formula in Lemma 3.5 and (3.12) implies that

$$\pi(\xi^r_{a,b}) = \Big(\sum_{\substack{\alpha\leq a\\ \beta\leq b}} c_{2^\alpha 32^\beta} - \sum_{\substack{\alpha\leq a\\ \beta< b}} c_{2^\beta 32^\alpha} + c_{12^r}\mathbb{I}(b\geq r) - c_{12^r}\mathbb{I}(a\geq r)\Big)\pi(\zeta^{\mathfrak{m}}(2r+1)),$$

where $1 \leq r \leq N$, and the sum is over $\alpha, \beta \geq 0$ satisfying $\alpha+\beta+1=r$. By induction hypothesis, and the fact that $c_{12^r} = 2(-1)^r$, the term in brackets is

$$2(-1)^r\Big[\sum_{\substack{\alpha\leq a\\ \beta\leq b}}\Big(A^r_{\alpha,\beta} - B^r_{\alpha,\beta}\Big) - \sum_{\substack{\alpha\leq a\\ \beta< b}}\Big(A^r_{\beta,\alpha} - B^r_{\beta,\alpha}\Big) + \mathbb{I}(b\geq r) - \mathbb{I}(a\geq r)\Big],$$

where all $\alpha+\beta+1=r$. By Lemma 4.2, this collapses to

$$2(-1)^r\Big(A^r_{a,b} - B^r_{a,b}\Big).$$

Putting the previous expressions together, we have shown that

$$D_{2r+1}\, \zeta^{\mathfrak{m}}(2^{\{a\}}32^{\{b\}}) = 2(-1)^r\Big(A^r_{a,b} - B^r_{a,b}\Big)\pi(\zeta^{\mathfrak{m}}(2r+1)) \otimes \zeta^{\mathfrak{m}}(2^{\{a+b+1-r\}}).$$

It follows by (3.3) and (3.9) that the difference

$$\Theta = \zeta^{\mathfrak{m}}(2^{\{a\}}32^{\{b\}}) - 2\sum_{r=1}^{a+b+1}(-1)^r(A^r_{a,b} - B^r_{a,b})\,\zeta^{\mathfrak{m}}(2r+1)\,\zeta^{\mathfrak{m}}(2^{\{a+b+1-r\}})$$

satisfies $D_{2r+1}\Theta = 0$ for all $r \leq a+b$. By Theorem 3.3, there is an $\alpha \in \mathbb{Q}$ such that

$$\Theta = \alpha\,\zeta^{\mathfrak{m}}(2a+2b+3).$$

Taking the period map implies an analogous relation for the ordinary multiple zeta values. By Theorem 4.1, the constant α is $2(-1)^{a+b+1}(A^{a+b+1}_{a,b} - B^{a+b+1}_{a,b})$, which completes the induction step, and hence the proof of the theorem. $\square$

4.2. 2-*adic properties of* c_w. The coefficients c_w satisfy some arithmetic properties which are crucial for the sequel, and follow immediately from Theorem 4.3.

Let p be a prime number. Recall that for any rational number $x \in \mathbb{Q}^\times$, its p-adic valuation $v_p(x)$ is the integer n such that $x = p^n\frac{a}{b}$, where a, b are relatively prime to p. We set $v_p(0) = \infty$. For any word $w \in \{2,3\}^\times$, let $\widetilde{w}$ denote the same word but written in reverse order.

COROLLARY 4.4. *Let w be any word of the form 2^a32^b of weight $2a+2b+3 = 2n+1$. It is obvious from formula* (4.2) *that $c_w \in \mathbb{Z}[\frac{1}{2}]$. Furthermore, the c_w satisfy*

(1) $c_w - c_{\widetilde{w}} \in 2\,\mathbb{Z}$,
(2) $v_2(c_{32^{a+b}}) \leq v_2(c_w) \leq 0$.

Proof. Property (1) follows from the symmetry $B^{a+b+1}_{a,b} = B^{a+b+1}_{b,a}$. Indeed,

$$c_{2^a32^b} - c_{2^b32^a} = \pm 2(A^{a+b+1}_{a,b} - A^{a+b+1}_{b,a}) \in 2\,\mathbb{Z}.$$

Let $n = a+b+1$ be fixed. Clearly, $v_2(c_{2^a32^b}) = v_2(2 \times 2^{-2n} \times \binom{2n}{2b+1})$, and so

$$v_2(c_{2^a32^b}) = 1 - 2n + v_2\Big(\binom{2n}{2b+1}\Big).$$

Writing $\binom{2n}{2b+1} = \frac{2n}{2b+1}\binom{2n-1}{2b}$, we obtain

$$v_2(c_{2^a32^b}) = 2 - 2n + v_2(n) + v_2\Big(\binom{2n-1}{2b}\Big)$$

which is ≤ 0, and furthermore, $v_2\Big(\binom{2n-1}{2b}\Big)$ is minimal when $b = 0$. This proves (2). $\square$

5. The level filtration and $\partial_{N,\ell}$ operators

Definition 5.1. Let $\mathcal{H}^{2,3} \subset \mathcal{H}$ denote the $\mathbb{Q}$-subspace spanned by

$$\zeta^{\mathfrak{m}}(w), \quad \text{where} \quad w \in \{2,3\}^\times. \tag{5.1}$$

It inherits the weight grading from $\mathcal{H}$. The weight of $\zeta^{\mathfrak{m}}(w)$ is $2\deg_2 w + 3\deg_3 w$.

Definition 5.2. Consider the unique map

$$\rho : \{2,3\}^{\times} \longrightarrow \{0,1\}^{\times} \tag{5.2}$$

such that $\rho(2) = 10$ and $\rho(3) = 100$, which respects the concatenation product. The motivic iterated integral which corresponds to $\zeta^{\mathfrak{m}}(w)$ is $I^{\mathfrak{m}}(0; \rho(w); 1)$.

LEMMA 5.3. *The coaction* (2.17) *gives a map*

$$\Delta : \mathcal{H}^{2,3} \longrightarrow \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}^{2,3}.$$

Proof. This follows from (2.18) together with the fact that $I^{\mathfrak{m}}$ vanishes on sequences which begin and end in the same symbol (I0). Thus, for $w \in \{2,3\}^{\times}$, every quotient sequence of $(0; \rho(w); 1)$ which occurs nontrivially on the right-hand side of the coaction is again of the form $(0; w'; 1)$, where w' is a word in 10 and 100. $\square$

5.1. *The level filtration.*

Definition 5.4. Let $w \in \{2,3\}^{\times}$ be a word in the letters 2 and 3. We define the *level* of w to be $\deg_3 w$, the number of occurrences of the letter '3' in w. Denote the induced increasing filtration on $\mathcal{H}^{2,3}$ by $F_{\bullet}$; i.e., $F_{\ell}\mathcal{H}^{2,3}$ is the $\mathbb{Q}$-vector space spanned by

$$\{\zeta^{\mathfrak{m}}(w) : w \in \{2,3\}^{\times} \text{ such that } \deg_3 w \leq \ell\}.$$

The empty word has level 0. The level counts the number of occurrences of the sequence '00' in $\rho(w)$. Alternatively, it is given by the weight minus twice the depth (number of 1's) in $\rho(w)$. Thus the level filtration takes even (resp. odd) values in even (resp. odd) weights. The level filtration is motivic in the following sense:

$$\Delta\Big(F_{\ell}\mathcal{H}^{2,3}\Big) \subseteq \mathcal{A} \otimes_{\mathbb{Q}} F_{\ell}\mathcal{H}^{2,3},$$

since any sequence of 0's and 1's contains at least as many '00's as any of its quotient sequences. It follows that the maps $D_{2r+1} : \mathcal{H}^{2,3} \to \mathcal{L}_{2r+1} \otimes_{\mathbb{Q}} \mathcal{H}^{2,3}$, where $\mathcal{L}$ is the Lie coalgebra of $\mathcal{A} = \mathcal{H}/f_2\mathcal{H}$, also preserve the level filtration. In fact, more is true.

LEMMA 5.5. *For all $r \geq 1$, $D_{2r+1}\Big(F_{\ell}\mathcal{H}^{2,3}\Big) \subseteq \mathcal{L}_{2r+1} \otimes_{\mathbb{Q}} F_{\ell-1}\mathcal{H}^{2,3}$.*

Proof. Let $w \in \{2,3\}^{\times}$ of level ℓ, so $\rho(w)$ contains exactly ℓ sequences 00. If a subsequence of odd length of $(0; \rho(w); 1)$ begins and ends in the same symbol, it is killed by $I^{\mathfrak{m}}$ by I0 and does not contribute to D_{2r+1}. Otherwise, it must necessarily contain at least one 00, and so the associated quotient sequence is of strictly smaller level. $\square$

Thus for all $r, \ell \geq 1$, we obtain a map

$$\mathrm{gr}_\ell^F D_{2r+1} : \mathrm{gr}_\ell^F \mathcal{H}^{2,3} \longrightarrow \mathcal{L}_{2r+1} \otimes_{\mathbb{Q}} \mathrm{gr}_{\ell-1}^F \mathcal{H}^{2,3}. \tag{5.3}$$

Note that Lemma 5.5 implies that $\mathcal{G}_{\mathcal{U}}$ respects the level filtration F and acts trivially on the associated graded. It follows that (5.3) factors through the one-dimensional subspace $[(\mathrm{Lie}\, \mathcal{G}_{\mathcal{U}})^{\mathrm{ab}}_{2r+1}]^\vee$ of $\mathcal{L}_{2r+1}$.

5.2. *The maps $\partial_{N,\ell}$.* In order to simplify notations, let us define $\zeta_{2r+1} \in \mathcal{L}_{2r+1}$ by

$$\zeta_{2r+1} = \pi(\zeta^{\mathfrak{m}}(2r+1)), \qquad \text{where } r \geq 1.$$

LEMMA 5.6. *Let $r, \ell \geq 1$. Then the map* (5.3) *satisfies*

$$\mathrm{gr}_\ell^F D_{2r+1}\Big(\mathrm{gr}_\ell^F \mathcal{H}^{2,3}\Big) \subseteq \mathbb{Q}\, \zeta_{2r+1} \otimes_{\mathbb{Q}} \mathrm{gr}_{\ell-1}^F \mathcal{H}^{2,3}.$$

Proof. Let $w \in \{2,3\}^\times$ of level ℓ, and let $I^{\mathfrak{m}}(0; \rho(w); 1)$ be the corresponding motivic iterated integral. From the definition of D_{2r+1}, we have

$$\mathrm{gr}_\ell^F D_{2r+1}(\zeta^{\mathfrak{m}}(w)) = \sum_\gamma \pi(I^{\mathfrak{m}}(\gamma)) \otimes \zeta^{\mathfrak{m}}(w_\gamma), \tag{5.4}$$

where the sum is over all subsequences γ of $(0; \rho(w); 1)$ of length $2r+1$, and w_γ is the corresponding quotient sequence. If γ contains more than one subsequence 00, then w_γ is of level $< \ell - 1$ and so does not contribute. If γ begins and ends in the same symbol, then $I^{\mathfrak{m}}(\gamma)$ is zero. One checks that $I^{\mathfrak{m}}(\gamma)$ can be of four remaining types:

(1) $I^{\mathfrak{m}}(0; 10\ldots 1\mathbf{00}10 \ldots 10; 1) = \zeta^{\mathfrak{m}}(2^{\{\alpha\}}32^{\{\beta\}})$,
(2) $I^{\mathfrak{m}}(1; 01\ldots 01\mathbf{00}1 \ldots 01; 0) = -\zeta^{\mathfrak{m}}(2^{\{\alpha\}}32^{\{\beta\}})$,
(3) $I^{\mathfrak{m}}(\mathbf{0}; \mathbf{0}1 \ldots 10; 1) = \zeta_1^{\mathfrak{m}}(2^{\{r\}})$,
(4) $I^{\mathfrak{m}}(1; 01 \ldots 1\mathbf{0}; \mathbf{0}) = -\zeta_1^{\mathfrak{m}}(2^{\{r\}})$.

By Corollary 3.6 and (3.8), in every case we have $\pi(I^{\mathfrak{m}}(\gamma)) \in \mathbb{Q}\, \zeta_{2r+1} \subset \mathcal{L}_{2r+1}$. The coefficient of ζ_{2r+1} in $\pi(I^{\mathfrak{m}}(\gamma))$ is either $\pm c_{2^\alpha 3 2^\beta}$ or $\pm c_{12^r}$. $\square$

Sending ζ_{2r+1} to 1 gives a canonical identification of 1-dimensional vector spaces:

$$\mathbb{Q}\, \zeta_{2r+1} \overset{\sim}{\longrightarrow} \mathbb{Q}. \tag{5.5}$$

Definition 5.7. For all $N, \ell \geq 1$, let $\partial_{N,\ell}$ be the linear map

$$\partial_{N,\ell} : \mathrm{gr}_\ell^F \mathcal{H}_N^{2,3} \longrightarrow \bigoplus_{1 < 2r+1 \leq N} \mathrm{gr}_{\ell-1}^F \mathcal{H}^{2,3}_{N-2r-1} \qquad \Big(= \mathrm{gr}_{\ell-1}^F \mathcal{H}^{2,3}_{<N-1} \Big)$$

defined by first applying

$$\bigoplus_{1 < 2r+1 \leq N} \mathrm{gr}_\ell^F D_{2r+1} \Big|_{\mathrm{gr}_\ell^F \mathcal{H}_N^{2,3}}$$

and then sending all ζ_{2r+1} to 1 via (5.5). Note that since $F_0\mathcal{H}_0^{2,3} = \mathcal{H}_0^{2,3}$, the case $2r+1 = N$ only plays a role when $\ell = 1$.

Our goal is to show that the maps $\partial_{N,\ell}$ are injective for $\ell \geq 1$.

5.3. *Matrix representation for $\partial_{N,\ell}$.*

Definition 5.8. Let $\ell \geq 1$, and let $B_{N,\ell}$ denote the set of words $w \in \{2,3\}^{\times}$ of weight N and level ℓ, in reverse lexicographic order for the ordering $3 < 2$. Note that as all words in $B_{N,\ell}$ have the same length, this is the same as the lexicographic order for the ordering $2 < 3$. Let $B'_{N,\ell}$ denote the set of words $w \in \{2,3\}^{\times}$ of all weights $\leq N-3$ (including the empty word if $\ell = 1$) and level $\ell - 1$, also in reverse lexicographic order.

If we write $N = 2m + 3\ell$, and if $\ell \geq 1$, then clearly

$$|B_{N,\ell}| = \binom{m+\ell}{\ell} = \sum_{0 \leq m' \leq m} \binom{m'+\ell-1}{\ell-1} = |B'_{N,\ell}|.$$

Define a set of words

$$S = \{w : w \in \{2,3\}^{\times} \text{ of level } 1\} \cup \{12^k : k \in \mathbb{N}\}. \tag{5.6}$$

Let $\ell \geq 1$, and let $w \in B_{N,\ell}$. By (5.4) and the proof of Lemma 5.6,

$$\partial_{N,\ell}\, \zeta^{\mathfrak{m}}(w) = \sum_{w' \in B'_{N,\ell}} f^w_{w'} \zeta^{\mathfrak{m}}(w'), \tag{5.7}$$

where $f^w_{w'}$ is a $\mathbb{Z}$-linear combination of numbers $c_{w''} \in \mathbb{Q}$ for $w'' \in S$.

Definition 5.9. For $\ell \geq 1$, let $M_{N,\ell}$ be the matrix $(f^w_{w'})_{w \in B_{N,\ell}, w' \in B'_{N,\ell}}$, where w corresponds to the rows, and w' the columns.

Note that we have not yet proved that the elements $\zeta^{\mathfrak{m}}(w)$ for $w \in B_{N,\ell}$ or $B'_{N,\ell}$ are linearly independent. Nonetheless, the transpose of the matrix $M_{N,\ell}$ represents the map $\partial_{N,\ell}$. (The reason for writing it this way round is purely aesthetic; see the example overleaf)

5.4. *Formal coefficients.* It is convenient to consider a formal version of the map (5.7) in which the coefficients $f^w_{w'}$ are replaced by symbols. Each matrix element $f^w_{w'}$ of $M_{N,\ell}$ is a linear combination of c_w, where $w \in S$. Therefore, let $\mathbb{Z}^{(S)}$ denote the free $\mathbb{Z}$-module generated by symbols C_w, where $w \in S$, and formally define a map

$$\partial^f_{N,\ell} : \mathrm{gr}^F_\ell \mathcal{H}^{2,3}_N \longrightarrow \mathbb{Z}^{(S)} \otimes_{\mathbb{Z}} \mathrm{gr}^F_{\ell-1} \mathcal{H}^{2,3}_{<N-1}$$

from the formula (5.4) by replacing the coefficient $\pm c_w$ of $\pi(I^{\mathfrak{m}}(\gamma))$ with its formal representative $\pm C_w$. Likewise, let $M^f_{N,\ell}$ be the matrix with coefficients in $\mathbb{Z}^{(S)}$ which is the formal version of $M_{N,\ell}$. There is a linear map

$$\mu : \mathbb{Z}^{(S)} \longrightarrow \mathbb{Q} \qquad (5.8)$$
$$C_w \mapsto c_w .$$

Then, by definition, $\partial_{N,\ell} = (\mu \otimes \mathrm{id}) \circ \partial^f_{N,\ell}$ and $M_{N,\ell}$ is obtained from the matrix $M^f_{N,\ell}$ by applying μ to all of its entries.

5.5. *Example.* In weight 10 and level 2, the matrix $M^f_{10,2}$ is as follows. The words in the first row (resp. column) are the elements of $B'_{10,2}$ (resp. $B_{10,2}$) in order.

	223	232	23	322	32	3
2233	C_3-C_{12}		$C_{23}-C_{32}-C_{122}$			$C_{223}-C_{322}$
2323		C_3-C_{12}	C_{23}			
2332			C_{32}	$C_{23}-C_{32}$		
3223	C_{12}		$C_{32}-C_{23}+C_{122}$	C_3-C_{12}	$C_{23}-C_{122}$	C_{322}
3232		C_{12}			C_{32}	C_{232}
3322				C_{12}	$C_{32}-C_{23}+C_{122}$	C_{322}

All blank entries are zero. Let us check the entry for

$$\zeta^{\mathfrak{m}}(3,3,2,2) = I^{\mathfrak{m}}(\underset{a_0}{0};\underset{a_1}{1}00100101\underset{a_{10}}{0};\underset{a_{11}}{1}).$$

Number the elements of the right-hand sequence $a_0, \ldots, a_{11}$ for reference, as shown. The nonvanishing terms in $\mathrm{gr}^F_2 D_3$ correspond to the subsequences commencing at a_0, a_1, a_3, a_4, a_5. They all give rise to the same quotient sequence, and we get

$$\begin{aligned}
&\pi(I^{\mathfrak{m}}(0;100;1)) \otimes I^{\mathfrak{m}}(0;1001010;1) + \pi(I^{\mathfrak{m}}(1;001;0)) \otimes I^{\mathfrak{m}}(0;1001010;1)\\
&\quad + \pi(I^{\mathfrak{m}}(0;100;1)) \otimes I^{\mathfrak{m}}(0;1001010;1) + \pi(I^{\mathfrak{m}}(1;001;0)) \otimes I^{\mathfrak{m}}(0;1001010;1)\\
&\quad + \pi(I^{\mathfrak{m}}(0;010;1)) \otimes I^{\mathfrak{m}}(0;1001010;1)
\end{aligned}$$

which gives $(C_3 - C_3 + C_3 - C_3 + C_{12})\,\zeta^{\mathfrak{m}}(3,2,2) = C_{12}\,\zeta^{\mathfrak{m}}(3,2,2)$. The nonzero terms in $\mathrm{gr}^F_2 D_5$ correspond to subsequences commencing at a_3, a_4, a_5. They give

$$\begin{aligned}
&\pi(I^{\mathfrak{m}}(0;10010;1)) \otimes I^{\mathfrak{m}}(0;10010;1) + \pi(I^{\mathfrak{m}}(1;00101;0)) \otimes I^{\mathfrak{m}}(0;10010;1)\\
&\qquad + \pi(I^{\mathfrak{m}}(0;01010;1)) \otimes I^{\mathfrak{m}}(0;10010;1)
\end{aligned}$$

which is $(C_{32} - C_{23} + C_{122})\,\zeta^{\mathfrak{m}}(3,2)$. Finally, the only nonzero term in $\mathrm{gr}^F_2 D_7$ corresponds to the subsequence commencing at a_3, giving

$$\pi(I^{\mathfrak{m}}(0;1001010;1)) \otimes I^{\mathfrak{m}}(0;100;1)$$

which is $C_{322}\,\zeta^{\mathfrak{m}}(3)$. The matrix $M_{10,2}$ is obtained by replacing each C_w by c_w.

6. Calculation of $\partial_{N,\ell}$

Let $I \subseteq \mathbb{Z}^{(S)}$ be the submodule spanned by elements of the form:

$$C_w - C_{\widetilde{w}} \text{ for } w \in \{2,3\}^\times \text{ of level } 1 \qquad \text{and} \qquad C_{12^k} \text{ for } k \in \mathbb{N}, \tag{6.1}$$

where $\widetilde{w}$ denotes the reversal of the word w. We show that modulo I the maps $\partial^f_{N,\ell}$ act by deconcatenation.

THEOREM 6.1. *Let w be a word in $\{2,3\}^\times$ of weight N, level ℓ. Then*

$$\partial^f_{N,\ell}\,\zeta^{\mathfrak{m}}(w) \equiv \sum_{\substack{w=uv \\ \deg_3 v=1}} C_v\,\zeta^{\mathfrak{m}}(u) \pmod{I},$$

where the sum is over all deconcatenations $w = uv$, where $u, v \in \{2,3\}^\times$, and where v is of level 1, *i.e., contains exactly one letter* '3'.

Proof. A subsequence of length $2r+1$ of the element $I^{\mathfrak{m}}(0;\rho(w);1)$ which corresponds to $\zeta^{\mathfrak{m}}(w)$ can be of the following types (compare the proof of Lemma 5.6):

(1) The subsequence is an alternating sequence of 1's and 0's, and does not contain any consecutive 0's. For reasons of parity, its first and last elements are equal. Thus by I0, this case does not contribute.

(2) The subsequence contains one set of consecutive 0's and is of the form $(0;w';1)$, where the inital 0 and final 1 are directly above the two arrows below:

$$\cdots 01\underset{\uparrow}{\mathbf{0}}\mathbf{0}10\cdots 1010\underset{\uparrow}{1}0\cdots\,.$$

The word w' consists of the $r+1$ symbols strictly in between the arrows. This subsequence corresponds to $I^{\mathfrak{m}}(\mathbf{0};\mathbf{0}10\ldots 10;1)$ which is $\zeta^{\mathfrak{m}}_1(2^{\{r\}})$. The contribution is therefore $C_{12^r} \in I$. With similar notations, the case

$$\cdots 0\underset{\uparrow}{1}0101\cdots 01\underset{\uparrow}{\mathbf{0}}\mathbf{0}10\cdots$$

corresponds to $I^{\mathfrak{m}}(1;01\ldots 01\mathbf{0};\mathbf{0})$ and contributes $-C_{12^r} \in I$, by relation I3.

(3) The subsequence is of one of two forms:

$$\underset{a}{0}\underset{b}{1}010\cdots 1\mathbf{00}\cdots 101\underset{a'}{1}\underset{b'}{0}$$

and contains exactly one set of consecutive 0's. The subsequence from a to a' is of the form $I^{\mathfrak{m}}(0;1010\ldots 1\mathbf{00}10\ldots 10;1)$ and contributes a $\zeta^{\mathfrak{m}}(2^{\{\alpha\}}32^{\{\beta\}})$. The subsequence from b to b' is of the form

$$I^{\mathfrak{m}}(1;010\ldots 1\mathbf{00}10\ldots 101;0).$$

Using relation I3, this contributes a $(-1)^{2r+1}\zeta^{\mathfrak{m}}(2^{\{\beta\}}32^{\{\alpha\}})$. Thus the total contribution of these two subsequences is

$$C_{2^\alpha 32^\beta} - C_{2^\beta 32^\alpha} \in I.$$

(4) The subsequence has at least two sets of consecutive 0's. This case does not contribute, since if the subsequence has level ≥ 2, the quotient sequence has level $\leq \ell - 2$ which maps to zero in $\mathrm{gr}^F_{\ell-1}\mathcal{H}^{2,3}$.

Thus every nontrivial subsequence is either of the form (2), or pairs up with its immediate neighbour to the right to give a contribution of type (3). The only remaining possibility is the final subsequence of $2r+1$ elements, which has no immediate right neighbour. This gives rise to a single contribution of the form

$$C_v \zeta^{\mathfrak{m}}(u),$$

where $w = uv$ and v has weight $2r+1$. If v has level strictly greater than 1, then by the same reasoning as (4) it does not contribute. This proves the theorem. □

Corollary 6.2. *The matrices $M^f_{N,\ell}$ modulo I are upper-triangular. Every entry which lies on the diagonal is of the form $C_{32^{r-1}}$, where $r \geq 1$, and every entry lying above it in the same column is of the form $C_{2^a 32^b}$, where $a+b+1=r$.*

Proof. Let $\ell \geq 1$ and consider the map

$$\begin{aligned} B'_{N,\ell-1} &\longrightarrow B_{N,\ell} \\ u &\mapsto u\,32^{\{r-1\}}, \end{aligned} \tag{6.2}$$

where $r \geq 1$ is the unique integer such that the weight of $u\,32^{\{r-1\}}$ is equal to N. This map is a bijection and preserves the ordering of both $B'_{N,\ell-1}$ and $B_{N,\ell}$. It follows from Theorem 6.1 that the diagonal entries of $M^f_{N,\ell}$ modulo I are of the form $C_{32^{r-1}}$. Now let $u \in B'_{N,\ell-1}$. All nonzero entries of $M^f_{N,\ell}$ modulo I in the column indexed by u lie in the rows indexed by $u2^{\{a\}}32^{\{b\}}$, where $a+b=r-1$. Since

$$u2^{\{a\}}32^{\{b\}} < u\,32^{\{r-1\}},$$

it is upper-triangular, and the entry in row $u2^{\{a\}}32^{\{b\}}$ and column u is $C_{2^a 32^b}$. □

7. Proof of the main theorem

7.1. *p-adic lemma.* We need the following elementary lemma.

LEMMA 7.1. *Let p be a prime, and let v_p denote the p-adic valuation. Let $A = (a_{ij})$ be a square $n \times n$ matrix with rational coefficients such that*

$$\text{(7.1)} \qquad \begin{aligned} &\text{(i)} \quad v_p(a_{ij}) \geq 1 \quad \textit{for all } i > j \\ &\text{(ii)} \quad v_p(a_{jj}) = \min_i \{v_p(a_{ij})\} \leq 0 \quad \textit{for all } j. \end{aligned}$$

Then A is invertible.

Proof. We show that the determinant of A is nonzero. The determinant is an alternating sum of products of elements of A, one taken from each row and column. Any such monomial $m \neq 0$ has k terms on or above the diagonal, in columns $j_1, \ldots, j_k$, and $n - k$ terms strictly below the diagonal. By (i) and (ii), its p-adic valuation is

$$v_p(m) \geq (n-k) + \sum_{r=1}^{k} v_p(a_{j_r j_r}).$$

If m is not the monomial m_0 in which all terms lie on the diagonal, then $k < n$, and

$$v_p(m) > \sum_{i=1}^{n} v_p(a_{ii}) = v_p(m_0).$$

It follows that $v_p(\det(A)) = v_p(m_0) = \sum_{i=1}^{n} v_p(a_{ii}) \leq 0 < \infty$, so $\det(A) \neq 0$. □

Remark 7.2. Another way to prove this lemma is simply to scale each column of the matrix A by a suitable power of p so that (i) remains true and so that the diagonal elements have valuation exactly equal to 0. The new matrix has p-integral coefficients by (ii), is upper-triangular mod p, and is invertible on the diagonal.

THEOREM 7.3. *For all $N, \ell \geq 1$, the matrices $M_{N,\ell}$ are invertible.*

Proof. We show that $M_{N,\ell}$ satisfies the conditions in (7.1) for $p = 2$. The entries of $M_{N,\ell}$ are deduced from those of $M^f_{N,\ell}$ by applying the map μ of (5.8). It follows from Corollary 4.4(1) and Lemma 3.8 that the generators (6.1) of I map to even integers under μ; i.e.,

$$\mu(I) \subset 2\,\mathbb{Z}.$$

By Corollary 6.2, this implies that $M_{N,\ell}$ satisfies (i). Property (ii) follows from Corollary 4.4(2), since the diagonal entries of $M^f_{N,\ell}$ mod I are C_{32^k}, $k \in \mathbb{N}$. □

7.2. *Proof of the main theorem.*

THEOREM 7.4. *The elements $\{\zeta^{\mathfrak{m}}(w) : w \in \{2,3\}^\times\}$ are linearly independent.*

Proof. By induction on the level. The elements of level zero are of the form $\zeta^{\mathfrak{m}}(2^{\{n\}})$ for $n \geq 0$, which by Lemma 3.4 are linearly independent. Now suppose that

$$\{\zeta^{\mathfrak{m}}(w) : w \in \{2,3\}^{\times}, \quad w \text{ of level } = \ell\}$$

are independent. Since the weight is a grading on the motivic multiple zeta values, we can assume that any nontrivial linear relation between the set of $\zeta^{\mathfrak{m}}(w)$ for $w \in \{2,3\}^{\times}$ of level $\ell+1$ is of homogeneous weight N. By Theorem 7.3, the map $\partial_{N,\ell+1}$ is injective and therefore gives a nontrivial relation of strictly smaller level, a contradiction. Thus $\{\zeta^{\mathfrak{m}}(w) : w \in \{2,3\}^{\times}$ of level $\ell+1\}$ are linearly independent, which completes the induction step. The fact that the operator $D_{\leq N}$ strictly decreases the level (Lemma 5.5), and that its level-graded pieces $\partial_{N,\ell}$ are injective, implies that there can be no nontrivial relations between elements $\zeta^{\mathfrak{m}}(w)$ of different levels. □

It follows that

$$\dim \mathcal{H}^{2,3}_N = \#\{w \in \{2,3\}^{\times} \text{ of weight } N\} = d_N, \tag{7.2}$$

where d_N is the dimension of $\mathcal{U}_N$ (2.23). The inclusions

$$\mathcal{H}^{2,3} \subseteq \mathcal{H} \subseteq \mathcal{H}^{\mathcal{MT}_+}$$

are therefore all equalities, since their dimensions in graded weight N are equal. The equality $\mathcal{H}^{2,3} = \mathcal{H}$ implies the following corollary.

Corollary 7.5. *Every motivic multiple zeta value $\zeta^{\mathfrak{m}}(a_1, \ldots, a_n)$ is a $\mathbb{Q}$-linear combination of $\zeta^{\mathfrak{m}}(w)$ for $w \in \{2,3\}^{\times}$.*

This implies Conjecture 2. The equality $\mathcal{H} = \mathcal{H}^{\mathcal{MT}_+}$ implies Conjecture 1.

8. A polynomial basis for motivic MZV's

Let X be a finite set which is equipped with a total ordering. Recall that a *Lyndon* word in X is an element w of $X^{\times}$ such that w is smaller than every strict right factor in the lexicographic ordering $w < v$ if $w = uv$ (concatenation), where $u, v \neq \emptyset$.

Let $X_{3,2} = \{2,3\}$ with the ordering $3 < 2$.

Theorem 8.1. *The set of elements*

$$\{\zeta^{\mathfrak{m}}(w), \text{ where } w \text{ is a Lyndon word in } X_{3,2}\}$$

form a polynomial basis for $\mathcal{H}$ (and hence $\mathcal{H}^{\mathcal{MT}_+}$).

By applying the period map, we obtain the following corollary.

Corollary 8.2. *Every multiple zeta value is a polynomial with coefficients in $\mathbb{Q}$ in*

$$\{\zeta(w), \text{ where } w \text{ is a Lyndon word in } X_{3,2}\}.$$

Remark 8.3. The theorem and its corollary are also true if one takes the alphabet $\{2,3\}$ with the ordering $2<3$. Other bases are possible: for example, by applying I3.

8.1. *Preliminary remarks.* Let $X=\{3,5,7,\ldots\}$ be the set of odd integers >1 with the usual ordering. Define the *weight* of a word $w\in X^\times$ to be the sum of all its letters and the *level* to be its length. The weight of $w\in X_{3,2}^\times$ is the sum of its letters and its level is the number of 3's. Let $\mathsf{Lyn}_{N,\ell}(X)$ (resp. $\mathsf{Lyn}_{N,\ell}(X_{3,2})$) denote the set of Lyndon words on X (resp. $X_{3,2}$) of weight N and level ℓ. Consider the map

$$\begin{aligned}\phi : X &\longrightarrow X_{3,2}\\ \phi(2n+1) \;&=\; 32^{\{n-1\}} \qquad \text{for } n\geq 1.\end{aligned} \tag{8.1}$$

It induces a map $\phi: X^\times \to X_{3,2}^\times$, which preserves the weight and level.

LEMMA 8.4. *It induces a bijection* $\phi:\mathsf{Lyn}_{N,\ell}(X)\to\mathsf{Lyn}_{N,\ell}(X_{3,2})$ *for all* $N\geq 3, \ell\geq 1$.

Proof. This is a standard property of Lyndon words and follows from the definition. □

Finally, let $\mathsf{Lie}(X)$ denote the free Lie algebra over $\mathbb{Q}$ generated by the elements of X. It shall be viewed as a subalgebra of the free associative algebra generated by X. There is a well-known map

$$\begin{aligned}\mathsf{Lyn}_{N,\ell}(X) &\longrightarrow \mathsf{Lie}(X)\\ w \;&\mapsto\; \lambda_w,\end{aligned} \tag{8.2}$$

such that the elements λ_w, as w ranges over the set of all Lyndon words in X, form a basis for $\mathsf{Lie}(X)$. To define λ, one uses the fact that a Lyndon word w of length ≥ 2 has a standard factorization $w=uv$, where u and v are Lyndon and v is the strict right Lyndon factor of w of maximal length. Inductively define $\lambda_w=w$ if w is a single letter and $\lambda_w=[\lambda_u,\lambda_v]$ if $w=uv$ is the standard factorization of w.

The main property of this map (see, e.g., [3, eq. (2.2.1)]) is that

$$\lambda_w = w + \text{ terms which are strictly greater than } w. \tag{8.3}$$

8.2. *Proof of Theorem* 8.1. Throughout, let $N\geq 3,\ell\geq 1$. Consider the map

$$\begin{aligned}\rho:\mathsf{Lyn}_{N,\ell}(X) &\longrightarrow \mathrm{gr}^F_\ell\mathcal{H}^{2,3}_N\\ w \;&\mapsto\; \zeta^{\mathfrak{m}}(\phi(w))\end{aligned} \tag{8.4}$$

which, to every Lyndon word in X, associates a motivic multiple zeta value. By Lemma 8.4, its argument is a Lyndon word in $X_{3,2}$.

For all $r \geq 1$, let $\partial_{2r+1} : \mathrm{gr}^F_\ell \mathcal{H}^{2,3}_N \to \mathrm{gr}^F_{\ell-1}\mathcal{H}^{2,3}_{N-2r-1}$ denote the corresponding piece of the map $\partial_{N,\ell}$ of Definition 5.7, and ∂^f_{2r+1} its formal version (the corresponding piece of the map $\partial^f_{N,\ell}$ defined in §5.4) . Let $w \in X^\times_{3,2}$. By Theorem 6.1, we have

$$\partial^f_{2r+1}\zeta^{\mathfrak{m}}(w) \equiv C_v \zeta^{\mathfrak{m}}(u) \pmod{I}, \tag{8.5}$$

if $w = uv$, where v is of level 1 and weight $2r+1$, and $\partial^f_{2r+1}\zeta^{\mathfrak{m}}(w) \equiv 0 \pmod{I}$ otherwise. Consider the unique morphism of monoids $\partial : X^\times \to \{\partial_3, \partial_5, \ldots\}^\times$ which sends the letter $2n+1$ to ∂_{2n+1}. There is a corresponding formal version where we replace ∂_{2n+1} by ∂^f_{2n+1}. By composing this map with (8.2), we obtain a map

$$\sigma : \mathsf{Lyn}_{N,\ell}(X) \longrightarrow \mathsf{Lie}(\partial_3, \partial_5, \ldots), \tag{8.6}$$

which sends every Lyndon word in X to a derivation on $\mathrm{gr}^F_\ell \mathcal{H}^{2,3}$. Consider the pairing

$$\begin{aligned} \mathsf{Lyn}_{N,\ell}(X) \times \mathsf{Lyn}_{N,\ell}(X) &\to \mathbb{Q} \\ (w, w') &\mapsto \sigma_w \circ \rho(w'), \end{aligned} \tag{8.7}$$

and let $P_{N,\ell}$ denote the square matrix whose rows and columns are indexed by $\mathsf{Lyn}_{N,\ell}(X)$, ordered lexicographically, with entries $\sigma_w \circ \rho(w')$. To compute $P_{N,\ell}$, let $w, w' \in X^\times$ and write $w' = (2i_1+3)\ldots(2i_\ell+3)$, where $i_k \geq 0$. From (8.5), one checks that

$$\partial^f_w \zeta^{\mathfrak{m}}(\phi(w')) \equiv \left\{ \begin{array}{ll} 0 & \text{if } w > w' \\ C_{32^{i_1}} \ldots C_{32^{i_\ell}} & \text{if } w = w' \\ 0 \text{ or } C_{2^{a_1}32^{b_1}} \ldots C_{2^{a_\ell}32^{b_\ell}} & \text{if } w < w' \end{array} \right\} \pmod{I}, \tag{8.8}$$

where a_k, b_k are some nonnegative integers satisfying $a_k + b_k = i_k$ for $1 \leq k \leq \ell$. It follows from (8.3), (8.8), and Corollary 4.4 that Lemma 7.1 applies to $P_{N,\ell}$, and therefore it is invertible. The image of the map (8.4) is spanned by the elements

$$A_{N,\ell} = \{\zeta^{\mathfrak{m}}(w) : w \in \mathsf{Lyn}_{N,\ell}(X_{3,2})\} \subset \mathrm{gr}^F_\ell \mathcal{H}^{2,3}_N .$$

Recall that $\mathcal{L}$ is the Lie coalgebra of $\mathcal{A} = \mathcal{H}/\zeta^{\mathfrak{m}}(2)\mathcal{H}$ and $\pi : \mathcal{H}_{>0} \to \mathcal{L}$ is the quotient map. Since the elements $\sigma_w \in \mathsf{Lie}(\partial_3, \partial_5, \ldots)$ kill products, the invertibility of $P_{N,\ell}$ implies that the image of the Lyndon elements $\pi(A_{N,\ell})$ are a basis of $\mathrm{gr}^F_\ell \mathcal{L}_N$ for $\ell \geq 1$ and $N \geq 3$. Since 2 is a Lyndon word in $X_{3,2}$, and $\zeta^{\mathfrak{m}}(2)$ is transcendental over $\mathcal{A}$, this proves that the elements $\zeta^{\mathfrak{m}}(w)$, for w a Lyndon word in $X_{3,2}$, are algebraically independent, and completes the proof. To prove Remark 8.3, repeat this argument with X replaced by $\{3, 5, 7, \ldots\}$ in reverse order, with the set $\{2, 3\}$ in the order $2 < 3$ instead of $X_{3,2}$, and replacing the map ϕ with the one which sends $2n+1$ to $2^{\{n-1\}}3$.

Example 8.5. In weight 20, level 2, $\mathsf{Lyn}_{20,2}(X) = \{3.17, 5.15, 7.13, 9.11\}$, where a dot denotes the concatenation product of letters in X. Thus $\sigma(a.b) = [\partial_a, \partial_b]$. The elements $A_{20,2}$ are of the form $\zeta^{\mathfrak{m}}(32^{\{a\}}32^{\{b\}})$, where $a+b=7$ and $0 \leq a \leq 3$. The formal version of the transpose matrix $P_{20,2}$, taken modulo I, is given by

	$[\partial_3, \partial_{17}]$	$[\partial_5, \partial_{15}]$	$[\partial_7, \partial_{13}]$	$[\partial_9, \partial_{11}]$
332222222	$C_3 C_{32^7}$	0	0	0
323222222	$C_3 C_{232^6}$	$C_{32} C_{32^6}$	0	0
322322222	$C_3 C_{2^2 32^5}$	$C_{32} C_{232^5}$	$C_{322} C_{32^5}$	0
322232222	$C_3 C_{2^3 32^4}$	$C_{32} C_{2^2 32^4}$	$C_{322} C_{232^4}$	$C_{32^3} C_{32^4}$

9. **Remarks**

It might be interesting to try to use the matrices $M_{N,\ell}$ to compute the multiplication law on the basis (1.2).

The geometric meaning of Theorem 4.3 is not clear. The term

$$(1 - 2^{-2r})\zeta(2r+1)$$

which comes from $B_r^{a,b}$ can be interpreted as an alternating sum and suggests that the formula should be viewed as an identity between motivic iterated integrals on $\mathbb{P}^1 \backslash \{0, \pm 1, \infty\}$. It would be interesting to find a direct motivic proof of Theorem 4.3 along these lines. Apart from the final step of Section 7.2, the only other place where we use the structure of the category $\mathcal{MT}(\mathbb{Z})$ is in Theorem 4.3. A proof of Theorem 4.3 using standard relations would give a purely combinatorial proof that $\dim \mathcal{H}_N \geq d_N$.

The argument in this paper could be dualized to take place in Ihara's algebra, using his pre-Lie operator ([4, eq. (5.13.5)]) instead of Goncharov's formula (2.18). This sheds some light on the appearance of the deconcatenation coproduct in Theorem 6.1.

Finally, we should point out that the existence of a different explicit basis for multiple zeta values was apparently announced many years ago by J. Ecalle.

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