RELATIONS AMONG MULTIPLE ZETA VALUES AND MODULAR FORMS OF LOW LEVEL

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May 9, 2016

DEDICATION

I dedicate this thesis

to my parents,

Genxiang and Ying,

and to my wife,

Luoman.

I love you all.

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ABSTRACT

This thesis explores various connections between multiple zeta values and modular forms of low level.

In the first part, we consider double zeta values of odd weight. We generalize a result of Gangl, Kaneko and Zagier on period polynomial relations among double zeta values of even weights to this setting. This answers a question asked by Zagier in [36]. We also prove a conjecture of Zagier on the inverse of a certain matrix in this setting.

In the second part, we study multiple zeta values of higher depth. In particular, we give a criterion and a conjectural criterion for "fake" relations in depth 4.

In the last part, we consider multiple zeta values of levels 2 and 3. We describe one connection with the Hecke operators T_2 and T_3, and another connection with newforms of level 2 and 3. We also give a conjectural generalization of the Eichler-Shimura-Manin correspondence to the spaces of newforms of levels 2 and 3.

CHAPTER 1

Introduction

1.1 Background

1.1.1 Background

A multiple zeta value (MZV) is a real number of the form

$$\zeta(n_1, \ldots, n_r) = \sum_{0<k_1<\cdots<k_r} \frac{1}{k_1^{n_1} \cdots k_r^{n_r}},$$

where $n_1, \ldots, n_{r-1} \geq 1$, $n_r \geq 2$ are integers. The weight of $\zeta(n_1, \ldots, n_r)$ is the quantity $n_1 + \cdots + n_r$, and its depth is r. These numbers were first defined by Euler for $r = 2$ in late 1700's, and they were popularized by Zagier in the 90's, who discovered numerous interesting relations they satisfy. Later, Hoffman made several conjectures about the structure of the MZVs in [19], and since then they have been the subject of extensive research.

MZVs occur in connection with Kontsevich's multiple integral defining an invariant of knots and links, and in Drinfeld's work on quantum groups. They also appear in quantum field theory and many other areas in modern mathematics. But for me, the most exciting thing about MZVs is the appearance of exotic relations such as

$$28\zeta(3,9) + 150\zeta(5,7) + 168\zeta(7,5) = \frac{5197}{691}\zeta(12). \tag{1.1.1}$$

It is the first in an infinite series of relations among double zeta values of even weight k discovered by Gangl, Kaneko and Zagier in [14]. Such relations are considered modulo a rational multiple of $\zeta(k)$. The coefficients of any of these relations can be computed by the coefficients of the even period polynomial of some cusp form of weight k for $\mathrm{SL}_2(\mathbb{Z})$, which gives a first direct connection between linear relations among double zeta values of weight k and the space of cusp forms of weight k.

1.1.2 What is new?

In this thesis, I have focused on extending the connection between MZVs and modular forms. My results include:

- In Theorem 5.1.2, I prove a conjecture of Zagier (cf. [36]) about the inverse matrix of a matrix related to (motivic) double zeta values of parity (even, odd). I introduce the idea of associating a homogenous polynomial with a vector to regard such a matrix as an operator on the space of homogenous polynomials. Then the main part of the proof can be done by using induction on the degrees of the associated polynomials. Later, such idea is generalized to depth 3 in [29].

- In Corollary 5.3.4, I obtain a family of Bernoulli number identities extending Carlitz's famous symmetric one. This family of Bernoulli number identities is closely related to the structure of double zeta values of odd weight.

- In Corollaries 5.4.1 and 5.4.2, I prove two families of standard relations between (motivic) double zeta values of odd weight k. The proofs of those two statements use the properties of the associated polynomial, which is basically the main step in the proof of Theorem 5.1.2.

- In Theorems 6.1.1 and 6.1.2, I prove two generalizations of Gangl-Kaneko-Zagier's result to the case of (motivic) double zeta values of parity (odd, even), which together answer a question asked by Zagier in [36]. The proofs use the relation between the left and the right annihilator of a certain matrix, which generalizes the idea of Gangl-Kaneko-Zagier in [14] and Baumard-Schneps in [1]. In Gangl-Kaneko-Zagier's formula (3.2.4), every coefficient is a single number, while in our formulas (6.1.1) and (6.1.2), every coefficient is a difference of two numbers.

- In Section 7.2, I give a generalization $\mathcal{C}^I_{k,r}$ of Brown's matrix $\mathcal{C}_{k,r}$ to (motivic) MZVs of arbitrary parity. Here k is the weight, r is the depth, and I is a r-tuple of positive integers of sum k. In Brown's work, I is taken to be the totally odd indexing set. In lower depth (depth ≤ 3), every element in the right annihilator of such a matrix will give us a linear relation between MZVs with indices in the set I.

- In Section 7.7, I give a criterion and a conjectural criterion for when a "relation" in depth 4 is "fake" (indeed not a relation). The conjectural criterion uses Conjecture 7.6.2, which gives a conjectural answer to a question asked by Brown in [7].

- In Section 8.3, I give two generalizations $\mathcal{C}^N_{k,r}$ and $\mathcal{D}^N_{k,r} \cdot \mathcal{C}^N_{k,r}$ of $\mathcal{C}_{k,r}$ to (motivic)

MZVs of depth $r = 2$ and levels $N = 2, 3$.

- In Theorem 8.4.2, I prove an analogue for $N = 2, 3$ of a result of Baumard and Schneps for $N = 1$ on the connection between the left annihilator of $\mathcal{C}^N_{k,2}$ and the periods of cusp forms for $\mathrm{SL}_2(\mathbb{Z})$. In this result, we see a connection with the Hecke operator T_N which is not seen for $N = 1$ since $T_1 = 1$. I also provide an algorithm to compute the eigenvalues and eigenforms for the Hecke operators T_2 and T_3. This provides evidence of the existence of a much deeper connection between MZVs and modular forms, not only in the level 1 case which has already been studied by many different people.

- Using $\mathcal{D}^N_{k,2} \cdot \mathcal{C}^N_{k,2}$, in Theorem 8.4.3, I prove a connection with the space of newforms of level $\Gamma_1(N)$ for $N = 2, 3$, which is also a higher-level analogue of Baumard and Schneps' result. In this result, we see the appearance of the Hecke operator U_N on newforms for $\Gamma_1(N)$ (see (8.4.6)). I also give a conjectural generalization of the Eichler-Shimura-Manin correspondence to $\Gamma_1(2)$ and $\Gamma_1(3)$. This provides additional evidence of the existence of a much deeper connection between MZVs and modular forms.

1.2 A brief description of the main results

1.2.1 Motivic double zeta values of parity (even,odd)

In [36], Zagier conjectured that the inverse of a matrix $\mathcal{A}$ corresponding to the parity (even, odd) double zeta values of weight $k = 2K + 1$ has two explicit expressions, which will be proved in this thesis. This matrix $\mathcal{A}$ comes from the decomposition formula of double zeta values of odd weight into a linear combination of products of two single zeta values. This is stated as the following theorem.

Theorem A. *For any odd integer $k = 2K + 1 \geq 5$, the matrix $\mathcal{A} := \mathcal{A}_k$ defined in (4.4.2), and for $1 \leq s, r \leq K - 1$, we have*

$$\left(\mathcal{A}^{-1}\right)_{r,s} = \frac{-2}{2s-1} \sum_{n=0}^{k-2s} \binom{k-2r-1}{k-2s-n} \binom{n+2s-2}{n} B_n \tag{1.2.1}$$

$$= \frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{2r-1}{k-2s-n} \binom{n+2s-2}{n} B_n, \tag{1.2.2}$$

This theorem gives us, as a corollary, for any $k = 2K+1$ and any $1 \leq r, s \leq K-1$, the following families of Bernoulli number identities.

Corollary. *Let $k = 2K + 1 \geq 5$ be an odd integer. For any integers r, s satisfying $1 \leq r, s \leq K - 1$, we have the following Bernoulli number identity*

$$\sum_{n=0}^{k-2s} \binom{2r-1}{k-2s-n} \binom{n+2s-2}{n} B_n = -\sum_{n=0}^{k-2s} \binom{k-2r-1}{k-2s-n} \binom{n+2s-2}{n} B_n. \tag{1.2.3}$$

When $s = 1$, this family is nothing but the following famous identity found by Carlitz [8] and proved by Shannon [33]:

$$(-1)^m \sum_{k=0}^{m} \binom{m}{k} B_{n+k} = (-1)^n \sum_{k=0}^{n} \binom{n}{k} B_{m+k}. \tag{1.2.4}$$

This result is important in understanding the space of double zeta values of odd weight k, as asserted by Zagier in [36]. By using the binomial coefficients of negative arguments defined by Kronenburg in [23], I also extended the above family (1.2.4) to

(5.3.10), where (1.2.4) itself is the special case when $i = 2r - 1$ with $1 \leq r \leq K - 1$ and $1 \leq s \leq K - 1$.

We can derive from this two families of standard relations between double zeta values of odd weight.

Corollary. *For any odd integer $k \geq 5$, we have the following relation*

$$\sum_{\substack{r+s=k \\ r:\text{even}}} (r-s)\zeta(r,s) + (2-k)\zeta(1,k-1) = \frac{k-7}{4}\zeta(k). \tag{1.2.5}$$

Corollary. *For any odd integer $k \geq 5$, we have the following relation*

$$(k-2)\zeta(k-2,2) + \sum_{\substack{r+s=k \\ 3\leq r\leq k-4:\text{odd}}} (r-s)\zeta(r,s) - 2(k-2)\zeta(1,k-1) = \frac{3(k-3)}{4}\zeta(k). \tag{1.2.6}$$

Both of these two corollaries also hold for motivic double zeta values, as we will see in Section 5.4.

1.2.2 Motivic double zeta values of parity (odd,even)

In his Annals paper [36], Zagier found an infinite series of relations between double zeta values of odd weight k and asked a question about whether there is an analogous connection to the cusp forms of weight $k \pm 1$ for $\mathrm{SL}_2(\mathbb{Z})$. In this thesis, we prove the following results, which give a complete answer to Zagier's question. They are analogues of the relations of Gangl-Kaneko-Zagier for the double zeta values of odd weight. One result uses odd period polynomials of cusp forms, while the other one uses restricted even period polynomials (see Section 2.2.1 for the notation). They can be stated as:

Theorem B (Type I)**.** *Let $k \geq 12$ be an even integer. To each odd period polynomial p of weight k, we associate the coefficients $b_{r,s}$ $(r+s=k+1)$ which are defined by*

$$p(X+Y,Y) = \sum_{r+s=k+1} \binom{k-1}{r-1} b_{r,s} X^{r-1} Y^{s-2}.$$

Then

$$\sum_{\substack{r+s=k+1 \\ 4\leq r\leq k-2:\text{even}}} (b_{r,s} - b_{s,r})\zeta(s,r) \equiv 0 \qquad (\text{mod } \zeta^{\mathfrak{m}}(k+1)). \tag{1.2.7}$$

Theorem C (Type II)**.** *Let $k \geq 12$ be an even integer. To each restricted (i.e., with X^{k-2} and Y^{k-2} terms removed) even period polynomial p of weight k, we associate the coefficients $c_{r,s}$ $(r+s=k-1)$ which are defined by*

$$\frac{\partial}{\partial X} p(X+Y,Y) = \sum_{r+s=k-1} \binom{k-3}{r-1} c_{r,s} X^{r-1} Y^{s-1}.$$

Then

$$\sum_{\substack{r+s=k-1 \\ 4\leq r\leq k-4:\text{even}}} (c_{r,s} - c_{s,r})\zeta(s,r) \equiv 0 \qquad (\text{mod } \zeta^{\mathfrak{m}}(k-1)). \tag{1.2.8}$$

Both of these two theorems also hold for motivic double zeta values, as we will see in Section 6.4.

1.2.3 Motivic MZVs of higher depth and fake relations

When all $n_1, \ldots, n_r$ are odd, we call the corresponding MZV totally odd. In the double zeta value case, we know from [14] that for a given even weight, the totally odd double zeta values generate the space of all MZVs of that weight. A few years ago, Francis Brown defined a family of matrices in [4] using the Ihara coaction and conjectured that we can use the right annihilators of these matrices to find all the relations between totally odd depth-graded motivic MZVs of any depth r. This family extends the depth 2 even weight case considered by Gangl, Kaneko, Zagier in [14] and Baumard, Schneps in [1]. In [35], Koji Tasaka gave a closed formula that expresses these matrices as products of $r-1$ square matrices, each of which only involves binomial coefficients. When the weight k and depth r satisfy $k \equiv r \pmod 2$, we extend the definition of such matrices to motivic MZVs of weight k and depth r, and we give a closed formula that is similar to Tasaka's.

In our setting, the right annihilators contain certain elements that do not give us linear relations between depth-graded motivic MZVs. We call such elements fake relations. The number of linearly independent fake relations was conjectured to be the dimension of the space of the cusp forms of weight k for $\mathrm{SL}_2(\mathbb{Z})$, and this is typically regarded as the first interesting case of the Broadhurst-Kreimer conjecture. In this thesis, we will give two criteria for a relation to be fake, and they will use two elements $\bar{\mathfrak{e}}$ and $\mathfrak{c}$ defined by Brown. We also give a reason why the fake relations appear.

1.2.4 Motivic MZVs of level 2, 3, Hecke operators, and newforms

MZVs of level N are generalizations of MZVs defined by

$$\zeta\binom{n_1, \dots, n_r}{\varepsilon_1, \dots, \varepsilon_r} = \sum_{0<k_1<\cdots<k_r} \frac{\varepsilon_1^{k_1} \cdots \varepsilon_r^{k_r}}{k_1^{n_1} \cdots k_r^{n_r}},$$

where ε_j is an Nth root of unity for each $j = 1, \dots, r$. As in the case of MZVs, the weight is $n_1 + \cdots + n_r$, and the depth is r. The integer N is called the level. Deligne

[10] has recently proved results for MZVs of level $N = 2, 3, 4, 6, 8$ that are analogous to the result $\mathcal{H}^{\mathcal{MT}} \cong \mathcal{H}$ in level 1 proved by Brown in [6]. The situation is rather different for such MZVs, since for these values of N, exotic relations such as (1.1.1) do not arise.

Although those exotic relations do not appear, the connection between MZVs of level N and cusp forms was expected by many people. In this thesis, we generalize Brown's matrix to the case of level $N = 2, 3$ and depth $r = 2$. We use this matrix $\mathcal{C}^N_{k,2}$ to determine the relations between such MZVs of level N. The disappearance of the exotic relations makes finding a connection with cusp forms a little more difficult at the beginning. However, we realized that there is a very nice connection between the matrix of level N defined here and the Hecke operator T_N of the cusp forms for $\mathrm{SL}_2(\mathbb{Z})$. By using our matrix, we can easily compute the periods of T_N-eigenforms, as well as T_N-eigenvalues. The appearance of Hecke operators in the picture of MZVs of level N seems to be totally new.

Theorem D (Connection with Hecke operators)**.** *Let k be an even integer. When $N = 2, 3$, the vectors coming from the restricted even period polynomials of cuspidal eigenforms of weight k for $\mathrm{SL}_2(\mathbb{Z})$ are left eigenvectors of $\mathcal{C}^N_{k,2}$, and the corresponding eigenvalues are given by*

- $N = 2$,

$$\frac{\lambda_2 - (1 + 2^{k-1})}{2^{k-2}},$$

- $N = 3$,

$$\frac{\lambda_3 - (1 + 3^{k-1})}{4 \cdot 3^{k-2}},$$

where λ_2 *(respectively,* λ_3*) is the eigenvalue for the Hecke operator* T_2 *(respectively,* T_3*) of the corresponding eigenform.*

Not only there is a connection between MZVs and the Hecke operators on $\mathrm{SL}_2(\mathbb{Z})$, but there is also a connection between another matrix, which is the product of a diagonal matrix $\mathcal{D}_{k,2}^N$ with $\mathcal{C}_{k,2}^N$, and the space of newforms of level $\Gamma_1(N)$.

Theorem E (Connection with newforms)**.** *Let* k *be an even integer. When* $N = 2, 3$*, the vectors coming from the restricted even period polynomials of newforms of weight* k *and level* $\Gamma_1(N)$ *are left eigenvectors of* $(\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N)$*, and the corresponding eigenvalues are given by*

- $N = 2$,
$$-\left(1 + \frac{\varepsilon}{2^{\frac{k-2}{2}}}\right),$$
- $N = 3$,
$$-\frac{1}{2}\left(1 + \frac{\varepsilon}{3^{\frac{k-2}{2}}}\right),$$

where the $\varepsilon = \pm 1$ *are the eigenvalues of the Atkin-Lehner involution of the corresponding newform.*

The proof of the above theorem leads us to the following conjectural analogue of the Eichler-Shimura-Manin correspondence for the newform spaces $\mathcal{S}_k^{\mathrm{new}}(\Gamma_1(2))^{\pm}$ and $\mathcal{S}_k^{\mathrm{new}}(\Gamma_1(3))^{\pm}$, where the sign $\pm$ indicates that we are considering on which the Atkin-Lehner involution acts by ± 1.

Conjecture F (Eichler-Shimura-Manin correspondence for $\mathcal{S}_k^{\text{new}}(\Gamma_1(2))^{\pm}$ and $\mathcal{S}_k^{\text{new}}(\Gamma_1(3))^{\pm}$)**.** *We have the following isomorphisms defined over* $\mathbb{C}$*:*

$$\mathcal{S}_k^{\text{new}}(\Gamma_1(2))^{\pm} \cong (\mathbf{W}_{2,\text{new}}^{-,0})^{\pm} := \left\{ p(x,y) \in \mathbb{C}[x,y] \;\middle|\; \begin{smallmatrix} 1) & -p(y,x)-p(y,x+y)+p(x,x+y)=-p(x,y) \\ 2) & -p(y,2x)=\pm 2^{\frac{k-2}{2}} p(x,y) \end{smallmatrix} \right\},$$

$$\mathcal{S}_k^{\text{new}}(\Gamma_1(3))^{\pm} \cong (\mathbf{W}_{3,\text{new},\pm}^{-,0})^{\pm} := \left\{ p(x,y) \in \mathbb{C}[x,y] \;\middle|\; \begin{smallmatrix} 1) & -p(y,x)-p(y,x+y)+p(x,x+y) \\ & -p(y,x-y)+p(x,x-y)=-p(x,y) \\ 2) & -p(y,3x)=\pm 3^{\frac{k-2}{2}} p(x,y) \end{smallmatrix} \right\}.$$

CHAPTER 2

Review of Modular Forms, Period Polynomials and Hecke Operators

2.1 Modular forms and cusp forms

2.1.1 Definition

In this section, we provide some background on modular forms. First, we introduce congruence subgroups.

Definition 2.1.1 (Principal congruence subgroup $\Gamma(N)$)**.** Let N be a positive integer. The principal congruence subgroup of level N is defined by

$$\Gamma(N) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}) : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \pmod{N} \right\}.$$

Definition 2.1.2 (Congruence subgroup)**.** A subgroup Γ of $\mathrm{SL}_2(\mathbb{Z})$ is called a congruence subgroup if $\Gamma(N) \subset \Gamma$ for some $N \in \mathbb{Z}^+$, in which case Γ is called a congruence subgroup of level N.

Example 2.1.3 ($\Gamma_0(N)$ and $\Gamma_1(N)$)**.** Besides the principal congruence subgroups, the most important congruence subgroups are

$$\begin{aligned} \Gamma_0(N) &= \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}) : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \begin{pmatrix} * & * \\ 0 & * \end{pmatrix} \pmod{N} \right\}, \\ \Gamma_1(N) &= \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}) : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \begin{pmatrix} 1 & * \\ 0 & 1 \end{pmatrix} \pmod{N} \right\}, \end{aligned}$$

where "$*$" means "unspecified".

Before giving the definition of modular forms, we need an operator called the weight k operator. The upper half plane is

$$\mathbb{H} = \{\tau \in \mathbb{C} : \mathrm{Im}(\tau) > 0\}.$$

Every element of $\mathrm{GL}_2^+(\mathbb{Q})$ can be viewed as an automorphism of the Riemann sphere $\widehat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$ known as the fractional linear transformation

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}(\tau) = \frac{a\tau + b}{c\tau + d}, \quad \tau \in \widehat{\mathbb{C}}. \tag{2.1.1}$$

From the definition, if $\gamma \in \mathrm{GL}_2^+(\mathbb{Q})$ and $\tau \in \mathbb{H}$ then $\gamma(\tau) \in \mathbb{H}$ as well.

Definition 2.1.4 (weight k operator)**.** For any $\gamma = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{GL}_2^+(\mathbb{Q})$ and for any integer k, define the weight k operator $[\gamma]_k$ on functions $f : \mathbb{H} \to \mathbb{C}$ by

$$(f|_k\gamma)(\tau) = \det(\gamma)^{k-1} j(\gamma,\tau)^{-k} f(\gamma(\tau)), \quad \tau \in \mathbb{H},$$

where

$$j(\gamma,\tau) = c\tau + d$$

is the factor of automorphy. In particular, when $\gamma \in \mathrm{SL}_2(\mathbb{Z})$, we have

$$(f|_k\gamma)(\tau) = j(\gamma,\tau)^{-k} f(\gamma(\tau)), \quad \tau \in \mathbb{H}.$$

Each congruence subgroup Γ of $\mathrm{SL}_2(\mathbb{Z})$ contains a translation matrix of the form

$$\begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix} : \tau \mapsto \tau + h$$

for some minimal $h \in \mathbb{Z}^+$. Every function $f : \mathbb{H} \to \mathbb{C}$ that is weight k-invariant under Γ is therefore $h\mathbb{Z}$-periodic and thus has a corresponding function $g : D' \to \mathbb{C}$ where D' is the punctured unit disk. This function g satisfies $f(\tau) = g(q_h)$, where $q_h = e^{\frac{2\pi i \tau}{h}}$.

Definition 2.1.5 (holomorphic at ∞)**.** Define f as above to be holomorphic at ∞ if g extends holomorphically to $q_h = 0$.

If f is holomorphic at ∞, then f has a Fourier expansion

$$f(\tau) = \sum_{n=0}^{\infty} a_n q_h^n, \quad q_h = e^{\frac{2\pi i}{h}}.$$

Definition 2.1.6 (Modular forms and cusp forms of weight k with respect to Γ)**.** Let Γ be a congruence subgroup of $\mathrm{SL}_2(\mathbb{Z})$ and let k be an integer. A function $f : \mathbb{H} \to \mathbb{C}$ is a modular form of weight k with respect to Γ if

(1) f is holomorphic,

(2) f is weight k-invariant under Γ,

(3) $f|_k\alpha$ is holomorphic at ∞ for all $\alpha \in \mathrm{SL}_2(\mathbb{Z})$.

If in addition,

(4) the constant term in the Fourier expansion of $f|_k\alpha$ vanishes for all $\alpha \in \mathrm{SL}_2(\mathbb{Z})$,

then f is a cusp form of weight k with respect to Γ. The modular forms of weight k with respect to Γ are denoted $\mathcal{M}_k(\Gamma)$, and the cusp forms are denoted $\mathcal{S}_k(\Gamma)$. Both of these spaces are $\mathbb{C}$-vector spaces.

We next consider some examples of modular forms.

Example 2.1.7 (Eisenstein series of weight k)**.** Let $k > 2$ be an even integer. We define the Eisenstein series of weight k to be

$$G_k(\tau) = \sum_{(c,d)\in\mathbb{Z}^2-\{(0,0)\}} \frac{1}{(c\tau+d)^k}, \quad \tau \in \mathbb{H}. \tag{2.1.2}$$

This is a modular form of weight k and level $\mathrm{SL}_2(\mathbb{Z})$.

2.1.2 Oldforms and newforms

In this section, we will give the definitions of oldforms and newforms. We first introduce the modular curves $X(\Gamma)$ and $Y(\Gamma)$. Then we define the Petersson inner product on $\mathcal{S}_k(\Gamma)$ under which the oldform and newform spaces are orthogonal to each other.

Definition 2.1.8 (Modular curves $Y(N)$ and $X(N)$)**.** For any congruence subgroup Γ of $\mathrm{SL}_2(\mathbb{Z})$, the modular curve $Y(\Gamma)$ is defined as the quotient space of orbits under Γ,

$$Y(\Gamma) = \Gamma\backslash\mathbb{H} = \{\Gamma\tau : \tau \in \mathbb{H}\}.$$

Setting $\mathbb{H}^* = \mathbb{H} \cup \mathbb{Q} \cup \{\infty\}$, the modular curve $X(\Gamma)$ is defined to be the extended quotient

$$X(\Gamma) = \Gamma\backslash\mathbb{H}^*.$$

Under a certain topology, where the open neighborhoods of ∞ are $U_r := \{z \in \mathbb{H} \mid \mathrm{Im}(z) > r\} \cup \{\infty\}$ and open neighborhoods of $a \in \mathbb{Q}$ are γU_r with $\gamma \in \mathrm{SL}_2(\mathbb{Z})$

satisfying $\gamma(\infty) = a$, the modular curve $X(\Gamma)$ is the compactification of $Y(\Gamma)$. Moreover, we have the following theorem (cf. [12, Proposition 2.4.2]).

Proposition 2.1.9. *The modular curve $X(\Gamma)$ is Hausdorff, connected, and compact.*

Define the hyperbolic measure on the upper half plane,

$$d\mu(\tau) = \frac{dxdy}{y^2}, \quad \tau = x + iy \in \mathbb{H}.$$

This measure is invariant under the $\mathrm{SL}_2(\mathbb{Z})$-action of $\mathbb{H}$, i.e., $d\mu(\alpha(\tau)) = d\mu(\tau)$ for all $\alpha \in \mathrm{SL}_2(\mathbb{Z})$ and $\tau \in \mathbb{H}$. Under such a measure, the volume of $X(\Gamma)$ is

$$V_\Gamma = \int_{X(\Gamma)} d\mu(\tau).$$

By using this hyperbolic measure, we may define the Petersson inner product on $\mathcal{S}_k(\Gamma)$.

Definition 2.1.10 (Petersson inner product)**.** Let $\Gamma \subset \mathrm{SL}_2(\mathbb{Z})$ be a congruence subgroup. The Petersson inner product

$$\langle\ ,\ \rangle_\Gamma : \mathcal{S}_k(\Gamma) \times \mathcal{S}_k(\Gamma) \to \mathbb{C} \tag{2.1.3}$$

is given by the integral

$$\langle f, g\rangle_\Gamma = \frac{1}{V_\Gamma} \int_{X(\Gamma)} f(\tau)\overline{g(\tau)}\mathrm{Im}(\tau)^k d\mu(\tau). \tag{2.1.4}$$

Before introducing newforms, we first give the definition of oldforms, which are basically the forms coming from lower levels. The most trivial way to move between levels is to observe that if $M \mid N$ then $\mathcal{S}_k(\Gamma_1(M)) \subset \mathcal{S}_k(\Gamma_1(N))$. Another way to embed $\mathcal{S}_k(\Gamma_1(M))$ into $\mathcal{S}_k(\Gamma_1(N))$ is by composing with the multiplication-by-d map where d is any factor of $\frac{N}{M}$. For any such d, let

$$\alpha_d = \begin{pmatrix} d & 0 \\ 0 & 1 \end{pmatrix}$$

so that $(f|_k\alpha_d)(\tau) = d^{k-1}f(d\tau)$ for $f : \mathbb{H} \to \mathbb{C}$. The weight k operator α_d maps injectively from $\mathcal{S}_k(\Gamma_1(M))$ to $\mathcal{S}_k(\Gamma_1(N))$, lifting the level from M to N.

Definition 2.1.11 (oldforms and newforms of level N)**.** For each divisor d of N, let i_d be the map

$$i_d : (\mathcal{S}_k(\Gamma_1(Nd^{-1})))^2 \to \mathcal{S}_k(\Gamma_1(N))$$

given by

$$(f, g) \mapsto f + g|_k\alpha_d.$$

The subspace of oldforms at level N is

$$\mathcal{S}_k(\Gamma_1(N))^{\text{old}} = \sum_{\substack{p|N \\ \text{prime}}} i_p(\mathcal{S}_k(\Gamma_1(Np^{-1}))^2),$$

and the space of newforms of level N is the orthogonal complement with respect to the Petersson inner product, i.e.,

$$\mathcal{S}_k(\Gamma_1(N))^{\text{new}} = (\mathcal{S}_k(\Gamma_1(N))^{\text{old}})^{\perp}.$$

2.1.3 Dimension formula

In this section, we provide the structure of the ring of modular forms (cf. [12, Theorem 3.5.2]). As a consequence, we obtain the generating series of $\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$. Later, this generating series will appear in the Broadhurst-Kreimer conjecture.

Proposition 2.1.12 (Structure of modular forms and cusp forms of level $\mathrm{SL}_2(\mathbb{Z})$)**.** *The ring of modular forms $\mathcal{M}(\mathrm{SL}_2(\mathbb{Z})) = \bigoplus_{k\in\mathbb{Z}} \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))$ and the ideal of cusp forms $\mathcal{S}(\mathrm{SL}_2(\mathbb{Z})) = \bigoplus_{k\in\mathbb{Z}} \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ are a polynomial ring in two variables and a principal ideal,*

$$\mathcal{M}(\mathrm{SL}_2(\mathbb{Z})) = \mathbb{C}[G_4, G_6], \quad \mathcal{S}(\mathrm{SL}_2(\mathbb{Z})) = \Delta \cdot \mathcal{M}(\mathrm{SL}_2(\mathbb{Z}))$$

where

$$\Delta = (60G_4(\tau))^3 - 27(140G_6(\tau))^2 \in \mathcal{S}_{12}(\mathrm{SL}_2(\mathbb{Z}))$$

is the unique weight 12 *cusp form up to a scalar.*

Remark. The generating series of the dimensions of the space of weight k cusp forms is given by

$$\mathbb{S}(x) = \sum_{n=0}^{\infty} \dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))x^k = \frac{x^{12}}{(1-x^4)(1-x^6)}. \tag{2.1.5}$$

2.2 Period polynomial of cusp forms

2.2.1 Definition

In this section, we will introduce the period polynomial of a cusp form. We will also give a definition of the $\mathrm{GL}_2^+(\mathbb{Q})$-action on the space of homogeneous polynomials in 2-variables.

Definition 2.2.1 (period polynomial of a cusp form)**.** The period polynomial of a cusp form f of weight k and level $\mathrm{SL}_2(\mathbb{Z})$ is the homogeneous polynomial of degree $k-2$ defined by

$$r_f(X, Y) = \int_0^{i\infty} f(\tau)(\tau Y - X)^{k-2} d\tau. \tag{2.2.1}$$

We denote its odd and even degree parts by $r_f^+(X,Y)$ and $r_f^-(X,Y)$, respectively.

The period polynomials are exactly the homogeneous polynomials $r_f(X,Y)$ of degree $k-2$ satisfying the two relations

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

Definition 2.2.2 (Vector space of period polynomials of weight k and level 1)**.** For each even integer k, let $\mathbf{V}_k(\mathbb{C}) = \langle X^{r-1}Y^{s-1} \mid r+s=k \rangle_{\mathbb{C}}$ be the $\mathbb{C}$-vector space of homogeneous polynomials of degree $k-2$ in two variables. Let $\mathbf{W}_k(\mathbb{C}) \subset \mathbf{V}_k(\mathbb{C})$ be the subspace of polynomials satisfying the relations

$$P(X,Y) + P(-Y,X) = 0, \tag{2.2.2}$$

$$P(X,Y) + P(X-Y,X) + P(Y,Y-X) = 0. \tag{2.2.3}$$

Similarly, we can define $\mathbf{V}_k(\mathbb{Q})$ and $\mathbf{W}_k(\mathbb{Q})$ to be the corresponding $\mathbb{Q}$-vector spaces. We use $\mathbf{W}_k$ to denote either $\mathbf{W}_k(\mathbb{Q})$ or $\mathbf{W}_k(\mathbb{C})$. We call $P \in \mathbf{W}_k$ a period polynomial of weight k and level 1. This period polynomial space splits as the direct sum of subspaces $\mathbf{W}_k^+$ and $\mathbf{W}_k^-$ of polynomials with odd and even degrees, respectively. We call these odd and even period polynomials.

Remark (Period polynomial of Eisenstein series). There is also a notion of period polynomials of Eisenstein series of weight k and level 1 given by

$$P_k^-(X,Y) = X^{k-2} - Y^{k-2}, \tag{2.2.4}$$

$$P_k^+(X,Y) \quad = \sum_{\substack{-1\le n\le k-1\\ n:\text{odd}}} \frac{B_{n+1}}{(n+1)!}\frac{B_{k-n-1}}{(k-n-1)!}X^nY^{k-2-n}, \tag{2.2.5}$$

which was discovered by Zagier in [38]. It is clear that $P_k^-(X,Y)\in\mathbf{W}_k^-$. Note that in this case, the odd part $P_k^+(X,Y)$ is not a polynomial.

Definition 2.2.3 (Restricted even period polynomial)**.** Let $P\in\mathbf{W}_k^-$ be any even period polynomial. Its image in $\mathbf{W}_k^-/\langle X^{k-2}-Y^{k-2}\rangle$ is called its restricted even period polynomial. We always identify this image P^0 of P as a polynomial in $\mathbf{W}_k^-$ without X^{k-2} and Y^{k-2} terms. The resulting subspace of $\mathbf{W}_k^-$ of restricted even period polynomials of weight k is denoted $\mathbf{W}_k^{-,0}$.

Definition 2.2.4 ($\mathrm{GL}_2^+(\mathbb{Q})$-action on $\mathbf{V}_k$)**.** For any $\gamma=\left(\begin{smallmatrix}a&b\\c&d\end{smallmatrix}\right)\in\mathrm{GL}_2^+(\mathbb{Q})$, and for any integer k, define the action of γ on polynomials $P(X,Y)\in\mathbf{V}_k$ by

$$(P|\gamma)(X,Y)=P(aX+bY,cX+dY). \tag{2.2.6}$$

Remark. The above $\mathrm{GL}_2^+(\mathbb{Q})$-action on period polynomials is compatible with the $\mathrm{GL}_2^+(\mathbb{Q})$-action on cusp forms defined before (cf. [37, Section 6]), i.e., for any $f\in\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ and any $\gamma\in\mathrm{GL}_2^+(\mathbb{Q})$, we have

$$(r_f|\gamma)(X,Y)=(r_{f|_k\gamma})(X,Y).$$

Remark. We can also define the period polynomial of a cusp form f of weight k and level Γ using the same formula

$$r_f(X,Y)=\int_0^{i\infty} f(\tau)(\tau Y-X)^{k-2}d\tau. \tag{2.2.7}$$

But if $\Gamma \neq \mathrm{SL}_2(\mathbb{Z})$, the relations they satisfy will not be

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

anymore: see Theorem 2.2.6 and Conjecture 8.8.4 for more details.

From the definition of the $\mathrm{SL}_2(\mathbb{Z})$-action on modular forms and period polynomials, we can see that the scalar matrix $-I_2$ acts trivially in both cases. Therefore the $\mathrm{SL}_2(\mathbb{Z})$-action naturally induces an $\mathrm{PSL}_2(\mathbb{Z})$-action by the same formula. There are 5 important elements in $\mathrm{PSL}_2(\mathbb{Z})$ which will be used later.

$$\varepsilon = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \ U = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix},$$
$$T = US = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \ T' = U^2S = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

By using the above matrices, the space W_k of period polynomials can also be defined as

$$\mathbf{W}_k = \ker(1+S) \cap \ker(1+U+U^2) \subset \mathbf{V}_k. \tag{2.2.8}$$

2.2.2 Eichler-Shimura-Manin correspondence in level 1, 2

In this section, we will review the Eichler-Shimura-Manin correspondence in levels 1 and 2.

Theorem 2.2.5 (level 1 Eichler-Shimura-Manin correspondence)**.** *(1) The map*

$$r^+ : \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z})) \to \mathbf{W}_k^+(\mathbb{C}), \quad f \mapsto r_f^+(X,Y)$$

is an isomorphism over $\mathbb{C}$*.*

(2) The map

$$r^- : \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})) \to \mathbf{W}_k^-(\mathbb{C}), \quad f \mapsto r_f^-(X,Y)$$

is an isomorphism over $\mathbb{C}$*. Moreover, this isomorphism* r^- *induces an isomorphism*

$$r^{-,0} : \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z})) \to \mathbf{W}_k^{-,0}(\mathbb{C}), \quad f \mapsto r_f^{-,0}(X,Y).$$

There is also a generalization of the Eichler-Shimura-Manin correspondence to the level $\Gamma_0(2)$ case given by Kaneko and Tasaka in [22]. (One should compare with the work of Merel in arbitrary level [30].)

Recall that the group $\Gamma_0(2)$ is generated by two elements

$$T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \text{ and } M = \begin{pmatrix} -1 & -1 \\ 2 & 1 \end{pmatrix}.$$

Consider the subspace $\mathbf{W}_{k,2}$ of $\mathbf{V}_k$ defined by

$$\mathbf{W}_{k,2} = \left\{ P \in \mathbf{V}_k \;\middle|\; P - P|T + P|M - P|(TM) = 0 \right\}.$$

For a cusp form $f \in \mathcal{S}_k(\Gamma_0(2))$, the period polynomial $r_f(X,Y)$ defined by (2.2.7) lies in the space $\mathbf{W}_{k,2}(\mathbb{C})$. Now we consider the odd and even degree parts of $\mathbf{W}_{k,2}$ and denote them by $\mathbf{W}_{k,2}^+$ and $\mathbf{W}_{k,2}^-$ respectively. As before, let $\mathbf{W}_{k,2}^{-,0}$ denote the resulting subspace of $\mathbf{W}_{k,2}^-$ of even polynomials with X^{k-2} and Y^{k-2} terms removed. Then we have the following level 2 version of the Eichler-Shimura-Manin correspondence from [22, Theorem 4].

Theorem 2.2.6 (level 2 Eichler-Shimura-Manin correspondence)**.** *For even* k*, the two maps*

$$r^+ : \mathcal{S}_k(\Gamma_0(2)) \to \mathbf{W}_{k,2}^+(\mathbb{C}) \text{ and } r^{-,0} : \mathcal{S}_k(\Gamma_0(2)) \to \mathbf{W}_{k,2}^{-,0}(\mathbb{C})$$

are isomorphisms of vector spaces over $\mathbb{C}$*.*

2.2.3 Examples of period polynomials in level 1 and $\Gamma_0(2)$

In this section, we will provide some examples of (restricted) even, odd period polynomials of level 1 and 2.

Example 2.2.7 (even period polynomials of level 1)**.** The following are the unique (up to a scalar) even period polynomials of the cusp forms of the corresponding weight and level $\mathrm{SL}_2(\mathbb{Z})$.

$$\begin{aligned}
\text{weight 12:} \quad & \frac{36}{691}(X^{10}-Y^{10}) - (X^8Y^2 - 3X^6Y^4 + 3X^4Y^6 - X^2Y^8) \\
\text{weight 16:} \quad & \frac{360}{3617}(X^{14}-Y^{14}) - (2X^{12}Y^2 - 7X^{10}Y^4 + 11X^8Y^6 \\
& \qquad -11X^6Y^8 + 7X^4Y^{10} - 2X^2Y^{12}) \\
\text{weight 18:} \quad & \frac{18000}{43867}(X^{16}-Y^{16}) - (8X^{14}Y^2 - 25X^{12}Y^4 + 26X^{10}Y^6 \\
& \qquad -26X^6Y^{10} + 25X^4Y^{12} - 8X^2Y^{14})
\end{aligned}$$

Example 2.2.8 (restricted even period polynomials of level 1)**.** The following are the unique (up to a scalar) restricted even period polynomials of the cusp forms of the corresponding weight and level $\mathrm{SL}_2(\mathbb{Z})$.

$$\begin{aligned}
\text{weight 12:} \quad & X^8Y^2 - 3X^6Y^4 + 3X^4Y^6 - X^2Y^8 \\
\text{weight 16:} \quad & 2X^{12}Y^2 - 7X^{10}Y^4 + 11X^8Y^6 - 11X^6Y^8 + 7X^4Y^{10} - 2X^2Y^{12} \\
\text{weight 18:} \quad & 8X^{14}Y^2 - 25X^{12}Y^4 + 26X^{10}Y^6 - 26X^6Y^{10} + 25X^4Y^{12} - 8X^2Y^{14}
\end{aligned}$$

Example 2.2.9 (odd period polynomials of level 1)**.** The following are the unique (up to a scalar) odd period polynomials of the cusp forms of the corresponding weight and level $SL_2(\mathbb{Z})$.

weight 12: $4X^9Y^1 - 25X^7Y^3 + 42X^5Y^5 - 25X^3Y^7 + 4X^1Y^9$

weight 16: $36X^{13}Y^1 - 245X^{11}Y^3 + 539X^9Y^5 - 660X^7Y^7$
$+539X^5Y^9 - 245X^3Y^{11} + 36X^1Y^{13}$

weight 18: $24X^{15}Y^1 - 154X^{13}Y^3 + 273X^{11}Y^5 - 143X^9Y^7$
$-143X^7Y^9 + 273X^5Y^{11} - 154X^3Y^{13} + 24X^1Y^{15}$

Example 2.2.10 (restricted even period polynomials of level $\Gamma_0(2)$)**.** The following are the unique (up to a scalar) restricted even period polynomials of the cusp forms of the corresponding weight and level $\Gamma_0(2)$.

weight 8: $X^2Y^4 - 2X^4Y^2$

weight 10: $2X^2Y^6 - 7X^4Y^4 + 8X^6Y^2$

weight 12: $X^2Y^8 - 3X^4Y^6 + 3X^6Y^4 - X^8Y^2$
$X^4Y^6 - 5X^6Y^4 + 7X^8Y^2$

2.3 Hecke operators

2.3.1 Hecke operators acting on modular forms

In this section, we will review the definition of Hecke operators of modular forms, and we will also review the Atkin-Lehner involution.

Definition 2.3.1 (double coset operator)**.** For congruence subgroups Γ_1 and Γ_2 of $SL_2(\mathbb{Z})$ and $\alpha \in GL_2^+(\mathbb{Q})$, the weight k operator $[\Gamma_1\alpha\Gamma_2]$ takes functions $f \in \mathcal{M}_k(\Gamma_1)$

to

$$f|_k[\Gamma_1\alpha\Gamma_2] = \sum_j f|_k\beta_j,$$

where $\{\beta_j\}$ are the coset representatives, i.e., $\Gamma_1\alpha\Gamma_2 = \bigcup_j \Gamma_1\beta_j$ is a disjoint union.

The double coset operator is well defined, i.e., it is independent of how the β_j are chosen. It takes modular forms of level Γ_1 to modular forms of level Γ_2, and it also takes cusp forms to cusp forms.

Diamond operators and Hecke operators are two special kinds of double coset operators.

Definition 2.3.2 (diamond operator $\langle d\rangle$)**.** Let N be a positive integer. For any $d \in (\mathbb{Z}/N\mathbb{Z})^*$, the diamond operator $\langle d\rangle$ on $\mathcal{M}_k(\Gamma_1(N))$ is

$$\langle d\rangle : \mathcal{M}_k(\Gamma_1(N)) \to \mathcal{M}_k(\Gamma_1(N))$$

given by

$$\langle d\rangle f = f|_k\alpha \text{ for any } \alpha = \left(\begin{smallmatrix} a & b \\ c & \delta \end{smallmatrix}\right) \in \Gamma_0(N) \text{ with } \delta \equiv d \pmod N$$

Remark. This is no nontrivial diamond operator in levels $1, 2$, and 3.

Definition 2.3.3 (Hecke operator T_p)**.** Let N be a positive integer. Let

$$\alpha = \begin{pmatrix} 1 & 0 \\ 0 & p \end{pmatrix},$$

where p is a prime. The double coset operator $\Gamma_1(N)\alpha\Gamma_1(N)$ is denoted T_p. Thus

$$\begin{aligned} T_p : \mathcal{M}_k(\Gamma_1(N)) &\to \mathcal{M}_k(\Gamma_1(N)) \\ f &\mapsto T_pf := f|_k[\Gamma_1(N) \left(\begin{smallmatrix} 1 & 0 \\ 0 & p \end{smallmatrix}\right) \Gamma_1(N)]. \end{aligned}$$

Proposition 2.3.4 (coset representatives)**.** *Let N be a positive integer, and let p be a prime. The operator T_p on $\mathcal{M}_k(\Gamma_1(N))$ is given by*

$$T_p f = \begin{cases} \sum_{j=0}^{p-1} f|_k \left(\begin{smallmatrix} 1 & j \\ 0 & p \end{smallmatrix}\right) & \text{if } p \mid N \\ \sum_{j=0}^{p-1} f|_k \left(\begin{smallmatrix} 1 & j \\ 0 & p \end{smallmatrix}\right) + f|_k[\left(\begin{smallmatrix} m & n \\ N & p \end{smallmatrix}\right)\left(\begin{smallmatrix} p & 0 \\ 0 & 1 \end{smallmatrix}\right)] & \text{if } p \nmid N, \text{ where } mp - nN = 1. \end{cases}$$

We have defined the Hecke operators $\langle d \rangle$ and T_p for $d \in (\mathbb{Z}/N\mathbb{Z})^*$ and p prime. Now we want to extend the definitions to $\langle n \rangle$ and T_n for all $n \in \mathbb{Z}^+$.

For $n \in \mathbb{Z}^+$ with $(n, N) = 1$, $\langle n \rangle$ is the above-defined diamond operator for $n \pmod N$. For $n \in \mathbb{Z}^+$ with $(n, N) > 1$, define $\langle n \rangle = 0$, the zero operator on $\mathcal{M}_k(\Gamma_1(N))$.

To define T_n, set $T_1 = 1$ (the identity operator); T_p is already defined for primes p. For prime powers, define inductively

$$T_{p^r} = T_p T_{p^{r-1}} - p^{k-1}\langle p \rangle T_{p^{r-2}} \text{ for } r \geq 2.$$

Extend the definition multiplicatively to T_n for all n, i.e., if $n = \prod p_i^{e_i}$ is the prime number decomposition of n, define

$$T_n = \prod T_{p_i^{e_i}}.$$

Definition 2.3.5 (eigenform)**.** A nonzero modular form $f \in \mathcal{M}_k(\Gamma_1(N))$ that is a simultaneous eigenvector for the Hecke operators T_n and $\langle n \rangle$ for all $n \in \mathbb{Z}^+$ is a called a Hecke eigenform, or simply an eigenform.

Theorem 2.3.6 (basis of eigenforms)**.** *The space $\mathcal{S}_k(\Gamma_1(N))^{\text{new}}$ has an orthogonal basis consisting of eigenforms.*

Definition 2.3.7 (Atkin-Lehner involution)**.** The Atkin-Lehner involution W_N on $\mathcal{M}_k(\Gamma_1(N))$ is defined by

$$W_N(f) = N^{\frac{2-k}{2}} f|_k \left(\begin{smallmatrix} 0 & -1 \\ N & 0 \end{smallmatrix}\right).$$

Note that $W_N^2 = (-1)^k$ is an involution when k is even. In particular, W_N preserves $\mathcal{S}_k(\Gamma_1(N))$. For such an operator W_N and k even, we can decompose the space $\mathcal{S}_k(\Gamma_1(N))$ into two eigenspaces $\mathcal{S}_k(\Gamma_1(N))^{\pm}$ such that

$$\mathcal{S}_k(\Gamma_1(N))^{\pm} = \{f \in \mathcal{S}_k(\Gamma_1(N)) \mid W_N f = \pm f\}. \tag{2.3.1}$$

Remark. The Atkin-Lehner involution also gives a decompostion of the newform space as

$$\mathcal{S}_k(\Gamma_1(N))^{\text{new}} = \mathcal{S}_k(\Gamma_1(N))^{\text{new},+} \oplus \mathcal{S}_k(\Gamma_1(N))^{\text{new},-}. \tag{2.3.2}$$

2.3.2 Hecke operators acting on period polynomials

In this section, we will review the definition of the action of Hecke operators on the space of period polynomials.

Theorem 2.3.8 ([37, Theorem 2])**.** *Let n be a positive integer, f a cusp form of weight k and level* $\mathrm{SL}_2(\mathbb{Z})$*. Then*

$$r_{T_n f}(X,Y) = \sum_{\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)} r_f(aX+bY, cX+dY),$$

where the sum is over matrices $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ of determinant n satisfying the conditions

$$a > |c|,\ d > |b|,\ bc \le 0, \quad b = 0 \Rightarrow -\frac{a}{2} < c \le \frac{a}{2}, \quad c = 0 \Rightarrow -\frac{d}{2} < b \le \frac{d}{2}. \tag{2.3.3}$$

For each integer $n \geq 1$ define

$$\mathbf{Man}_n = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} : a, b, c, d \in \mathbb{Z}, ad - bc = n, a, b, c, d \text{ satisfy (2.3.3)} \right\}.$$

The above theorem asserts that the actions of the Hecke operator T_n on f and r_f are compatible, i.e., we have

$$T_n(r_f) := \sum_{M \in \mathbf{Man}_n} r_f | M = r_{T_n f}.$$

The following example will be used later in Section 8.5.

Example 2.3.9. For $n = 2, 3$, we have

$$\begin{aligned} \mathbf{Man}_2 &= \left\{ \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix} \right\}, \\ \mathbf{Man}_3 &= \left\{ \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}, \begin{pmatrix} 3 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 3 & 0 \\ -1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 3 \end{pmatrix}, \begin{pmatrix} 1 & -1 \\ 0 & 3 \end{pmatrix} \right\}. \end{aligned}$$

From [37, Section 6], we know that this set $\mathbf{Man}_n$ also gives us the corresponding actions on the even and odd period polynomials, i.e., we have

$$r^{\pm}_{T_n f} = \sum_{M \in \mathbf{Man}_n} r^{\pm}_f | M.$$

Since T_n preserves the subspace of $\mathbf{W}_k^-$ generated by $x^{k-2} - y^{k-2}$, it induces

$$r^{-,0}_{T_n f} = \sum_{M \in \mathbf{Man}_n} r^{-,0}_f | M$$

as polynomials in $\mathbf{W}_k^{-,0}$, i.e., modulo $x^{k-2} - y^{k-2}$.

CHAPTER 3

Review of Multiple Zeta Values (MZVs)

3.1 Introduction of MZVs

In this section, we will review two definitions of multiple zeta values, one using infinite sum and another using iterated integral. We will also give the famous Broadhurst-Kreimer conjecture at the end of this section.

3.1.1 Definition of MZVs

We begin this section with the definition of multiple zeta values.

Definition 3.1.1 (multiple zeta value)**.** A multiple zeta value (MZV) is a real number

$$\zeta(n_1, \ldots, n_r) = \sum_{0<k_1<\cdots<k_r} \frac{1}{k_1^{n_1} \cdots k_r^{n_r}},$$

for integers $n_1, \ldots, n_{r-1} \geq 1$ and $n_r \geq 2$. The number $n_1 + \cdots + n_r$ is called the weight, and the number r is called the depth. By convention, $\zeta(0) = -\frac{1}{2}$ is regarded as the only MZV of weight 0 and depth 0.

Remark. In the literature, there are two different conventions for MZVs. Most of the work in this field adopts the above definition, while in the past people usually used the definition

$$\zeta_{\text{old}}(n_1, \ldots, n_r) = \sum_{k_1>\cdots>k_r>0} \frac{1}{k_1^{n_1} \cdots k_r^{n_r}}.$$

It is easy to see that we have

$$\zeta(n_1, \ldots, n_r) = \zeta_{\text{old}}(n_r, \ldots, n_1).$$

In this paper, we use the convention in Definition 3.1.1, except for the case of formal double zeta values.

Definition 3.1.2 (MZV algebra)**.** Let $\mathcal{Z}$ be the MZV algebra $\bigoplus_{k\geq 0} \mathcal{Z}_k$, where $\mathcal{Z}_k$ is the $\mathbb{Q}$-vector space spanned by all MZVs of weight k. Let $\mathfrak{D}$ be the depth filtration on $\mathcal{Z}$ defined by

$$\mathfrak{D}_0\mathcal{Z} = \mathbb{Q} \subset \mathfrak{D}_1\mathcal{Z} \subset \cdots \subset \mathfrak{D}_r\mathcal{Z} := \langle \zeta(n_1, \ldots, n_j) : j \leq r \rangle_{\mathbb{Q}} \subset \cdots .$$

The MZV algebra becomes a filtered algebra under this depth filtration $\mathfrak{D}$.

A product of two MZVs can be expressible as a linear combination of MZVs of the same weight. We will give an exact formula below in (3.1.3). Therefore, $\mathcal{Z}$ is closed under multiplication.

Definition 3.1.3 (depth-graded MZV)**.** Define $\mathrm{gr}_r^{\mathfrak{D}} \mathcal{Z}_k = \mathfrak{D}_r\mathcal{Z}_k / \mathfrak{D}_{r-1}\mathcal{Z}_k$ and let $\mathrm{gr}^{\mathfrak{D}} \mathcal{Z}$ be the bigraded $\mathbb{Q}$-algebra $\mathrm{gr}^{\mathfrak{D}} \mathcal{Z} = \bigoplus_{k,r} \mathrm{gr}_r^{\mathfrak{D}} \mathcal{Z}_k$. The depth-graded MZV

$$\zeta_{\mathfrak{D}}(n_1, \ldots, n_r) \in \mathrm{gr}_r^{\mathfrak{D}} \mathcal{Z}$$

is given by the class of $\zeta(n_1, \ldots, n_r)$ modulo elements of lower depth.

MZVs can also be defined by using iterated integrals, and this notion is exactly what people generalize to the so-called motivic MZVs (see Section 4.1). Let M be a smooth manifold over $\mathbb{R}$. Let $\gamma : [0,1] \to M$ be a piecewise smooth path on M, and let $\omega_1, \ldots, \omega_n$ be smooth $\mathbb{C}$-valued 1-forms on M. Let us write

$$\gamma^*(\omega_i) = f_i(t)dt,$$

for the pullback of the forms ω_i to the interval $[0,1]$.

Definition 3.1.4 (iterated integral)**.** Define the iterated integral of $\omega_1, \ldots, \omega_n$ along γ to be

$$\int_\gamma \omega_1 \cdots \omega_n = \int_{0 \le t_1 \le \cdots \le t_n \le 1} f_1(t_1)dt_1 \cdots f_n(t_n)dt_n. \tag{3.1.1}$$

The empty integral ($n = 0$) is defined to be constant 1.

For $M = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ and $a_i \in \{0,1\}$, let

$$I(0; a_1, \ldots, a_n; 1) = \int_0^1 \omega_{a_1} \ldots \omega_{a_n},$$

where $\omega_0 = \frac{dz}{z}$ and $\omega_1 = \frac{dz}{1-z}$. We view $a_1, \ldots, a_n$ also as a word $a_1 \cdots a_n$ in $\{0,1\}$. Write

$$\begin{aligned} \rho : \mathbb{Z}^r_{\ge 1} &\to \text{words in } \{0,1\} \\ (n_1, \ldots, n_r) &\mapsto 10^{n_1 - 1} \cdots 10^{n_r - 1}. \end{aligned}$$

When $n_r \ge 2$, we have

$$I(0; \rho(n_1, \ldots, n_r); 1) = \zeta(n_1, \ldots, n_r). \tag{3.1.2}$$

Otherwise, we need to take a regularization. Since we will not discuss the regularization here, the detailed discussion can be found in [21]. The shuffle product of MZVs is defined by using this iterated integral definition, which gives us the following formula (cf. [21]).

Theorem 3.1.5. *Given 1-forms $\omega_1, \ldots, \omega_{r+s}$ one has*

$$\int_\gamma \omega_1 \ldots \omega_r \int_\gamma \omega_{r+1} \ldots \omega_{r+s} = \sum_{\sigma \in \Sigma(r,s)} \int_\gamma \omega_{\sigma(1)} \cdots \omega_{\sigma(r+s)}, \tag{3.1.3}$$

where $\Sigma(r,s)$ is the set of (r,s)-shuffles

$$\Sigma(r,s) = \{\sigma \in \mathfrak{S}_{r+s} : \sigma(1) < \cdots < \sigma(r) \text{ and } \sigma(r+1) < \cdots < \sigma(r+s)\}$$

and $\mathfrak{S}_t$ is the symmetric group on t letters.

3.1.2 Broadhurst-Kreimer conjecture

Based on extensive computer calculations, Broadhurst and Kreimer [3] made a conjecture on the Poincaré series for the number of multiple zeta values of given weight and depth. Using the above notation for depth-graded MZVs, their conjecture can be stated as the following.

Conjecture 3.1.6 (Broadhurst-Kreimer conjecture)**.** *The generating series of the dimensions of the spaces $\mathrm{gr}_r^{\mathfrak{D}} \mathcal{Z}_k$ is given by*

$$\sum_{k,r \geq 0} \dim_{\mathbb{Q}}(\mathrm{gr}_r^{\mathfrak{D}} \mathcal{Z}_k) x^k y^r = \frac{1 + \mathbb{E}(x) y}{1 - \mathbb{O}(x) y + \mathbb{S}(x) y^2 - \mathbb{S}(x) y^4}, \tag{3.1.4}$$

where

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

The interpretation of $\mathbb{S}(x)$ as the generating series for the dimensions of the spaces of cusp forms of level $\mathrm{SL}_2(\mathbb{Z})$ is due to Zagier [39].

We call $\zeta_{\mathfrak{D}}(n_1, \ldots, n_r)$ a totally odd MZV when all n_i are odd and at least 3. The $\mathbb{Q}$-vector subspace of $\mathrm{gr}_r^{\mathfrak{D}} \mathcal{Z}_k$ spanned by all totally odd MZVs of weight k and depth r is denoted by $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{Z}_k^{\mathrm{odd}}$. As a convention, we set $\mathrm{gr}_0^{\mathfrak{D}}\mathcal{Z}_0^{\mathrm{odd}} = \mathbb{Q}$. Brown made the following totally odd Broadhurst-Kreimer conjecture [4, (10.4)].

Conjecture 3.1.7 (Totally odd Broadhurst-Kreimer conjecture)**.** *The generating series of the dimension of the spaces* $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{Z}_k^{\mathrm{odd}}$ *is given by*

$$\sum_{k,r\geq 0} \dim_{\mathbb{Q}}(\mathrm{gr}_r^{\mathfrak{D}}\mathcal{Z}_k^{\mathrm{odd}})x^k y^r = \frac{1}{1-\mathbb{O}(x)y+\mathbb{S}(x)y^2}, \tag{3.1.5}$$

where $\mathbb{E}(x)$, $\mathbb{O}(x)$, $\mathbb{S}(x)$ *are defined in Conjecture 3.1.6.*

3.2 Gangl-Kaneko-Zagier's result for formal double zeta values of even weight

In this section, we will review a result of Gangl, Kaneko and Zagier about the period polynomial relations between double zeta values of even weight.

3.2.1 Formal Double Zeta Value

We begin by reviewing the definition of the formal double zeta space (cf. [18], [21], [31]). Let $k > 2$ be an integer. We introduce formal variables $Z_{r,s}$, $P_{r,s}$ and Z_k and impose the relations

$$Z_{r,s} + Z_{s,r} = P_{r,s} - Z_k \qquad (r+s=k), \tag{3.2.1}$$

$$\sum_{r+s=k}\left[\binom{r-1}{i-1}+\binom{r-1}{j-1}\right]Z_{r,s} = P_{i,j} \qquad (i+j=k). \tag{3.2.2}$$

(From now on, whenever we write $r+s=k$ or $i+j=k$ without comment, it is assumed that the variables are integers ≥ 1.)

The formal double zeta space is defined as the $\mathbb{Q}$-vector space

$$\mathbf{D}_k = \frac{\{\mathbb{Q}\text{-linear combinations of formal symbols } Z_{r,s},\ P_{r,s},\ Z_k\}}{\langle \text{relations (3.2.1) and (3.2.2)}\rangle}. \tag{3.2.3}$$

The double zeta realization we consider in this paper is the following linear map $\mathbf{D}_k \to \mathbb{R}$ on the formal double zeta space:

$$Z_{r,s} \mapsto \begin{cases} \zeta(s,r), & \text{if } r > 1, \\ \kappa, & \text{if } r = 1, \end{cases}$$

$$P_{r,s} \mapsto \begin{cases} \zeta(r)\zeta(s), & \text{if } r, s > 1, \\ \kappa + \zeta(1, k-1) + \zeta(k), & \text{if } r = 1 \text{ or } s = 1, \end{cases}$$

$$Z_k \mapsto \zeta(k),$$

where $\kappa \in \mathbb{R}$ can be chosen to be any real number. Here the formal double zeta values are defined by generalizing the notion of double zeta values $\zeta_{\text{old}}(r, s)$. So when we are taking the double zeta realization, we translate the result into the convention $\zeta(s, r)$ instead of $\zeta_{\text{old}}(r, s)$.

Remark. There are also other realizations of formal double zeta values except for the above double zeta realization. For example, the author have constructed a so-called binomial realization in [28].

3.2.2 GKZ's Result in the formal double zeta value setting

One basic way of working with $\mathbf{D}_k$ is by studying the relations among the $Z_{r,s}$. Gangl, Kaneko and Zagier proved the following general result [14, Theorem 3] for the formal double zeta space $\mathbf{D}_k$. We denote by $\mathcal{P}_k^{\text{ev}}$ the subspace of $\mathbf{D}_k$ spanned by the $P_{\text{even,even}}$, i.e., the $P_{r,s}$ with r, s even. Let $\mathbf{W}_k^-(\mathbb{C})$ denote the $\mathbb{C}$-vector space of even period polynomials of weight k (see Section 2.2.1).

Theorem 3.2.1 (Gangl-Kaneko-Zagier)**.** *The spaces* $\mathcal{P}_k^{\mathrm{ev}}$ *and* $\mathbf{W}_k^-(\mathbb{C})$ *are canonically isomorphic to each other. More precisely, to each* $p \in \mathbf{W}_k^-(\mathbb{C})$ *we associate the coefficients* $p_{r,s}$ *and* $q_{r,s}$ $(r+s=k)$ *which are defined by* $p(X,Y) = \sum \binom{k-2}{r-1} p_{r,s} X^{r-1}Y^{s-1}$ *and* $p(X+Y,Y) = \sum \binom{k-2}{r-1} q_{r,s} X^{r-1}Y^{s-1}$. *Then* $q_{r,s} - q_{s,r} = p_{r,s}$ *(in particular* $q_{r,s} = q_{s,r}$ *for* r,s *even) and*

$$\sum_{\substack{r+s=k\\ r,s:\mathrm{even}}} q_{r,s} Z_{r,s} \equiv 3 \sum_{\substack{r+s=k\\ r,s:\mathrm{odd}}} q_{r,s} Z_{r,s} \qquad (\mathrm{mod}\ Z_k). \tag{3.2.4}$$

Conversely, an element $\sum_{r,s:\mathrm{odd}} c_{r,s} Z_{r,s} \in \mathbf{D}_k$ *belongs to* $\mathcal{P}_k^{\mathrm{ev}}$ *if and only if* $c_{r,s} = q_{r,s}$ *arising in this way.*

By taking the double zeta value realization, the following result for double zeta values [14, Theorem 3 (Rough statement)] follows directly.

Corollary 3.2.2. *The values* $\zeta(\mathrm{odd}, \mathrm{odd})$ *of weight* k *satisfy at least* $\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ $\mathbb{Q}$*-linearly independent relations.*

Gangl, Kaneko and Zagier also proved the following statement [14, Theorem 1].

Theorem 3.2.3 (Gangl-Kaneko-Zagier)**.** *For even* $k > 2$*, one has*

$$\sum_{\substack{r=2\\ r:\mathrm{even}}}^{k-1} Z_{r,k-r} = \frac{3}{4} Z_k, \qquad \sum_{\substack{r=2\\ r:\mathrm{odd}}}^{k-1} Z_{r,k-r} = \frac{1}{4} Z_k.$$

The double zeta value realization of the above statement tells us that for even $k > 2$, we always have

$$\sum_{\substack{r=2\\ r:\mathrm{even}}}^{k-1} \zeta(k-r, r) = \frac{3}{4}\zeta(k), \qquad \sum_{\substack{r=2\\ r:\mathrm{odd}}}^{k-1} \zeta(k-r, r) = \frac{1}{4}\zeta(k).$$

Remark. It is worth pointing out that the second identity is exactly the one obtained by Theorem 3.2.1 from the even period polynomial $X^{k-2} - Y^{k-2} \in \mathbf{W}_k^-$ of the Eisenstein series of weight k. Later, we will see that we cannot obtain any relations from the even period polynomials of Eisenstein series in the case of double zeta values of odd weight.

Remark. In Section 5.4, we construct two families of standard relations between double zeta values of parity (even, odd) and (odd, even), in which the numbers $\frac{1}{4}$ and $\frac{3}{4}$ also appear. The connection between these two appearances is still unknown to the author.

Example 3.2.4. For $k = 12$ and $k = 16$, the first two cases for which there are non-zero cusp forms of level $\mathrm{SL}_2(\mathbb{Z})$, we have the following identities:

$$\frac{5197}{691}\zeta(12) = 28\zeta(3,9) + 150\zeta(5,7) + 168\zeta(7,5),$$
$$\frac{78967}{3617}\zeta(16) = 66\zeta(3,13) + 375\zeta(5,11) + 686\zeta(7,9) + 675\zeta(9,7) + 396\zeta(11,5).$$

Remark. Note that 691 and 3617 are the irregular primes in the numerators of the Bernoulli numbers B_{12} and B_{16}.

3.3 Double zeta values of odd weight

In [36, Proposition 7], Zagier obtained the following relation, the existence of which was first predicted by Euler without the explicit formula in [13].

Proposition 3.3.1 (Zagier)**.** *The double zeta value $\zeta(m,n)$ $(m \geq 1, n \geq 2)$ of odd* *weight $m+n=k$ satisfies*

$$\zeta(m,n) = (-1)^m \sum_{s=0}^{\frac{k-3}{2}} \left[\binom{k-2s-1}{m-1} + \binom{k-2s-1}{n-1} - \delta_{n,2s} + (-1)^m \delta_{s,0} \right] \zeta(2s)\zeta(k-2s). \quad (3.3.1)$$

Remark. In Section 4.4.2, we will generalize this result to the motivic setting. In Chapters 5 and 6, we will prove several results related to this (motivic) decomposition formula.

CHAPTER 4

Review of Motivic MZVs

4.1 Motivic MZVs

The classical MZVs can be defined by using iterated integrals (see (3.1.2)). We define the motivic MZVs as motivic iterated integrals, which are the elements in the de Rham fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. Then we can define a graded algebra $\mathcal{H}$ whose image under a period map is the classical MZV algebra $\mathcal{Z}$. The coproduct structure on the motivic MZVs defined in Theorem 4.1.4 is a genuinely new feature given by the motivic theory, since it makes no sense to define such a coproduct structure on the level of MZVs because of the inaccessibility of the transcendence conjectures.

4.1.1 The Ihara action and the Ihara coaction

Let ${}_0\Pi_1$ be the de Rham fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ (cf. [11, Section 5.12]). It is the functor which to any $\mathbb{Q}$-algebra R associates the following subset of invertible formal power series in two non-commuting variables e_0 and e_1

$$ {}_0\Pi_1(R) = \{S \in R\langle\langle e_0, e_1\rangle\rangle^{\times} \mid \Delta(S) = S \otimes S\}, $$

where $R\langle\langle e_0, e_1\rangle\rangle$ denotes the formal power series ring in two non-commuting variables e_0 and e_1, and Δ is the unique R-algebra homomorphism satisfying

$\Delta(e_i) = 1 \otimes e_i + e_i \otimes 1$ for $i = 0, 1$. This ${}_0\Pi_1(R)$ is a group with the group law given by concatenation of series. It makes ${}_0\Pi_1$ a group scheme over $\mathbb{Q}$. The affine ring of ${}_0\Pi_1$ over $\mathbb{Q}$ is isomorphic to

$$\mathcal{O}({}_0\Pi_1) \cong \mathbb{Q}\langle e^0, e^1 \rangle, \tag{4.1.1}$$

where $\mathbb{Q}\langle e^0, e^1 \rangle$ denotes the polynomial ring in two non-commuting variables e^0 and e^1. The ring $\mathcal{O}({}_0\Pi_1)$ is a noncommutative, graded algebra equipped with the shuffle product. Here the grading on $\mathbb{Q}\langle e^0, e^1 \rangle$ is given by the length of the word, and the shuffle product ш is defined by

$$e^{i_1} \cdots e^{i_r} \text{ ш } e^{i_{r+1}} \cdots e^{i_{r+s}} = \sum_{\sigma \in \Sigma(r,s)} e^{i_{\sigma^{-1}(1)}} \cdots e^{i_{\sigma^{-1}(r+s)}},$$

where each i_j is either 0 or 1, and $\Sigma(r, s)$ is the set of σ in the symmetric group $\mathfrak{S}_{r+s}$ such that $\sigma(1) < \cdots < \sigma(r)$ and $\sigma(r+1) < \cdots < \sigma(r+s)$. Every word w in the letters e^0, e^1 corresponds to a unique function $w : {}_0\Pi_1(R) \to R$ 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.

There is a pro-unipotent group U^{dR} over $\mathbb{Q}$ acting on ${}_0\Pi_1$. Brown proved that its Lie algebra is free, generated by one element σ_{2n+1} in each degree $-2n-1$, for all $n \geq 1$ (cf. [6, Theorem 1.1]). We will not describe the action

$$U^{\mathrm{dR}} \times {}_0\Pi_1 \to {}_0\Pi_1$$

in detail. Instead, setting $\mathcal{A} = \mathcal{O}(U^{\mathrm{dR}})$, we will describe the corresponding coaction

$$\mathcal{O}({}_0\Pi_1) \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1), \tag{4.1.2}$$

since later the motivic MZVs will be defined as elements in a quotient of $\mathcal{O}({}_0\Pi_1)$ (cf. Definition 4.1.2). The structure of the Lie algebra of U^{dR} tells us that $\mathcal{A} \cong \mathbb{Q}\langle f_3, f_5, \ldots\rangle$ (see Section 4.1.5 for more details).

Remark. This U^{dR} is the unipotent part of G^{dR}, which is the motivic Galois group of the Tannakian category $\mathcal{MT}(\mathbb{Z})$ of the mixed Tate motives over $\mathbb{Z}$ with fibre functor being the de Rham realization. This category $\mathcal{MT}(\mathbb{Z})$ is explicitly constructed by Marc Levine (cf. [24]). In general, the motivic Galois group of a Tannakian category $\mathcal{M}$ is the group scheme G over $\mathbb{Q}$ which gives us an equivalence between $\mathcal{M}$ and the representation category of G. Such an equivalence of categories is a generalization of the usual Galois theory (0-dimensional case), which describes the equivalence of categories between finite separable extensions K of a field k and non-empty finite sets with a (continuous) transitive action of the absolute Galois group of k. The above action $U^{\mathrm{dR}} \times {}_0\Pi_1 \to {}_0\Pi_1$ is just the action induced by the G^{dR}-action $G^{\mathrm{dR}} \times {}_0\Pi_1 \to {}_0\Pi_1$.

Let A denote the group of automorphisms of ${}_0\Pi_1$. The action of U^{dR} on ${}_0\Pi_1$ factors through the action of A on ${}_0\Pi_1$. The latter action $A \times {}_0\Pi_1 \to {}_0\Pi_1$ was first computed by Ihara in the setting ${}_0\Pi_1 \times {}_0\Pi_1 \to {}_0\Pi_1$ via the isomorphism (cf. [11, Sections 5.9 and 5.15])

$$A \xrightarrow{\sim} {}_0\Pi_1, \quad a \mapsto a \cdot {}_0 1_1,$$

where ${}_0 1_1$ is the identity element in the group scheme ${}_0\Pi_1$.

Definition 4.1.1 (Ihara action and Ihara coaction)**.** The above action

$${}_0\Pi_1 \times {}_0\Pi_1 \to {}_0\Pi_1 \tag{4.1.3}$$

is called the Ihara action, and its dual coaction

$$\Delta : \mathcal{O}({}_0\Pi_1) \to \mathcal{O}({}_0\Pi_1) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1). \tag{4.1.4}$$

is called the Ihara coaction.

Remark. The coaction (4.1.2) is obtained by composing Δ of (4.1.4) with the map

$$a : \mathcal{O}({}_0\Pi_1) \to \mathcal{A}, \quad \phi \mapsto (g \mapsto \phi(g \cdot {}_01_1)), \tag{4.1.5}$$

applied to the left-hand factor of $\mathcal{O}({}_0\Pi_1) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1)$, i.e.,

$$\mathcal{O}({}_0\Pi_1) \xrightarrow{\Delta} \mathcal{O}({}_0\Pi_1) \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1) \xrightarrow{a\otimes \mathrm{id}} \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{O}({}_0\Pi_1).$$

The image $a(\phi) = (g \mapsto \phi(g \cdot {}_01_1))$ is an element in $\mathcal{A} = \mathcal{O}(U^{\mathrm{dR}})$, since $g \cdot {}_01_1 \in {}_0\Pi_1$ for any $g \in U^{\mathrm{dR}}$.

In Theorem 4.1.4, we will give an explicit formula for an action induced from (4.1.5), which suffices for the purposes of this thesis. We denote the coaction (4.1.2) also by Δ.

Let $\mathrm{dch} \in {}_0\Pi_1(\mathbb{R})$ be the element

$$\mathrm{dch} = \sum_{i_j \in \{0,1\}} e_{i_1} \cdots e_{i_n} \int_\gamma \omega_{i_1} \cdots \omega_{i_n},$$

where γ is the line segment from 0 to 1, $\omega_0 = \frac{dt}{t}$ and $\omega_1 = \frac{dt}{1-t}$. When $i_1 \neq 1$ or $i_n \neq 0$, the integral must be regularized for the reasons of convergence (cf. [21]), but we will not discuss this here. The coefficients of words beginning with e_1 and ending in e_0 are the MZVs, and dch is known as the Drinfeld associator. The first few terms of dch (the terms of shortest word length) are

$$\mathrm{dch} = 1 + \zeta(2)[e_1, e_0] + \zeta(3)[e_0, [e_0, e_1]] + \zeta(1,2)[e_1, [e_1, e_0]] + \cdots . \tag{4.1.6}$$

Evaluation at dch is a homomorphism

$$\mathrm{dch} : \mathcal{O}({}_0\Pi_1) \to \mathbb{R} \tag{4.1.7}$$

which maps a word $w \in \mathcal{O}({}_0\Pi_1)$ in e^0, e^1 to the coefficient of the corresponding word (changing e^i to e_i) in dch.

4.1.2 Motivic MZVs

Let $I \subset \mathcal{O}({}_0\Pi_1)$ be the kernel of the map (4.1.7). It describes the $\mathbb{Q}$-linear relations between MZVs. For example,

$$\zeta(3) = \zeta(1,2) \Longleftrightarrow e^1e^0e^0 - e^1e^1e^0 \in I.$$

Let $J^{\mathcal{MT}} \subseteq I$ be the largest graded ideal contained in I which is stable under the coaction (4.1.2), i.e., $\Delta(J^{\mathcal{MT}}) \subseteq \mathcal{A} \otimes J^{\mathcal{MT}} + J^{\mathcal{MT}}\mathcal{A} \otimes \mathcal{O}({}_0\Pi_1)$, where $J^{\mathcal{MT}}$ acts on $\mathcal{A}$ via the map $\mathcal{O}({}_0\Pi_1) \to \mathcal{A}$ defined in (4.1.5).

Definition 4.1.2 (motivic MZV)**.** Define the graded coalgebra of motivic multiple zeta values (motivic MZVs) to be

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

By replacing i with e^i for $i = 0, 1$, a word w in the letters 0 and 1 represents a word consisting of e^0 and e^1, hence w defines an element in (4.1.1). Denote its image in $\mathcal{H}$ by

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

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

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

In the case when $n_0 = 0$, we simply write this as $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$ and call it a motivic MZV.

We call $n_0 + n_1 + \cdots + n_r$ the weight and r the depth of $\zeta^{\mathfrak{m}}_{n_0}(n_1, \ldots, n_r)$. The space $\mathcal{H}$ has the natural structure of a graded $\mathbb{Q}$-algebra, i.e.,

$$\mathcal{H} = \bigoplus_{k \geq 0} \mathcal{H}_k,$$

where $\mathcal{H}_k$ denotes the $\mathbb{Q}$-vector space spanned by all motivic MZVs of weight k. We also regard $\mathbb{Q}$ as the space of motivic MZVs of weight 0 and depth 0, and the product is naturally given by the shuffle product of iterated integrals, i.e., the shuffle product induced from $\mathcal{O}({}_0\Pi_1) \cong \mathbb{Q}\langle e^0, e^1 \rangle$.

Since $J^{\mathcal{MT}}$ is stable under the coaction (4.1.2), we have an induced coaction $\Delta : \mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$, i.e., the following diagram commutes:

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

Furthermore, the map dch (4.1.7) factors through $\mathcal{H}$ since $J^{\mathcal{MT}} \subseteq I = \ker(\mathrm{dch})$, which we denote by

$$\mathrm{per} : \mathcal{H} \to \mathbb{R}.$$

In particular, when $n_r \geq 2$, we have

$$\mathrm{per}(\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)) = \zeta(n_1, \ldots, n_r).$$

4.1.3 Properties of motivic iterated integrals

In this section, we describe the fundamental properties satisfied by motivic iterated integrals (see [6, Section 2.4]) for later reference. Previously, $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})$ has been only defined for $a_0 = 0$ and $a_{n+1} = 1$. By using the properties below, we can also define them for any $a_0, a_{n+1} \in \{0, 1\}$ and still call them motivic iterated integrals.

$\mathbf{I_0}$: 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 $a_1 = \cdots = a_n$.

$\mathbf{I_1}$: $I^{\mathfrak{m}}(a_0; a_1) = 1$ for all $a_0, a_1 \in \{0, 1\}$.

$\mathbf{I_2}$: *Shuffle product (special case).* For $k \geq 0$, $n_1, \ldots, n_r \geq 1$, we have

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

$\mathbf{I_3}$: *Reflection formula.* For all $a_1, \ldots, a_n \in \{0, 1\}$, we have

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

From $\mathbf{I_0}$ and $\mathbf{I_3}$, we can see that every nonzero motivic iterated integral can be written as one with $a_0 = 0$ and $a_{n+1} = 1$. Note that $\mathbf{I_2}$ is the special case of the motivic version of the shuffle product (3.1.3) with $s = 0$.

4.1.4 Coaction on the space $\mathcal{H}$

We begin this section with the following theorem due to Brown [6, Section 2.3].

Theorem 4.1.3 (Brown)**.** *There is an isomorphism of graded $\mathcal{A}$-comodules*

$$\mathcal{H} \cong \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)], \tag{4.1.8}$$

where $\Delta(\zeta^{\mathfrak{m}}(2)) = 1 \otimes \zeta^{\mathfrak{m}}(2)$. Moreover, this isomorphism is compatible with (4.1.5) in the sense that

$$\begin{array}{ccc} \mathcal{O}({}_0\Pi_1) & \longrightarrow & \mathcal{A} \\ \downarrow & & \uparrow \\ \mathcal{H} & \longrightarrow & \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)] \end{array}$$

commutes.

So from now on, we may regard $\mathcal{A}$ as the quotient algebra $\mathcal{H}/\zeta^{\mathfrak{m}}(2)\mathcal{H}$. Under this quotient map, let us denote by $I^{\mathfrak{a}}$ the image in the space $\mathcal{A}$ of the corresponding motivic iterated integral $I^{\mathfrak{m}}$. Using this notation, the coaction $\mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$ can be computed by the exactly same formula as in [16, Theorem 1.2] (with the factors interchanged).

Theorem 4.1.4 (Coaction for the motivic MZVs)**.** *If $a_0, \ldots, a_{n+1} \in \{0, 1\}$, then $\Delta I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})$ equals*

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

4.1.5 $\mathcal{A}$-comodule structure of the space $\mathcal{H}$

In this section, we will review a theorem proved by Brown, which describes the structure of $\mathcal{A}$ and $\mathcal{H}$. Let us consider the following noncommutative polynomial algebra over $\mathbb{Q}$ freely generated by symbols f_{2i+1} in weights $2i + 1$:

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

The vector space $\mathcal{U}'$ is equipped with an additional product given by the shuffle product ш

$$f_{i_1}\cdots f_{i_r} ш f_{i_{r+1}}\cdots f_{i_{r+s}} = \sum_{\sigma\in\Sigma(r,s)} f_{i_{\sigma^{-1}(1)}}\cdots f_{i_{\sigma^{-1}(r+s)}},$$

where $\Sigma(r,s)$ is as in Section 4.1.1. With respect to the shuffle product and the coproduct given by the deconcatenation map $\Delta^\bullet : \mathcal{U}' \to \mathcal{U}' \otimes_{\mathbb{Q}} \mathcal{U}'$ defined by

$$\Delta^\bullet(f_{i_1}\cdots f_{i_r}) = \sum_{j=0}^{r} f_{i_1}\cdots f_{i_j} \otimes f_{i_{j+1}}\cdots f_{i_r},$$

the vector space $\mathcal{U}'$ is a Hopf algebra. Let us consider the graded vector space

$$\mathcal{U} := \mathcal{U}' \otimes_{\mathbb{Q}} \mathbb{Q}[f_2] = \bigoplus_{k\geq 0} \mathcal{U}_k,$$

where f_2 is a commutative symbol of weight 2, and the graded part of $\mathcal{U}$ of weight k is denoted by $\mathcal{U}_k$. The space $\mathcal{U}$ carries a graded $\mathcal{U}'$-comodule structure, with the coaction $\Delta^\bullet : \mathcal{U} \to \mathcal{U}' \otimes \mathcal{U}$ satisfying $\Delta^\bullet(f_2) = 1 \otimes f_2$ and $\Delta^\bullet(wf_2^n) = \Delta^\bullet(w)\Delta^\bullet(f_2)^n$ for any $n > 0$ and $w \in \mathcal{U}'$. Let us further define

$$f_{2n} := \frac{\zeta^{\mathfrak{m}}(2n)}{\zeta^{\mathfrak{m}}(2)^n} f_2^n,$$

for $n \geq 1$. Here the quotient $\frac{\zeta^{\mathfrak{m}}(2n)}{\zeta^{\mathfrak{m}}(2)^n} = \frac{\zeta(2n)}{\zeta(2)^n}$ is a rational number. Since the Hoffman basis conjecture is true for motivic multiple zeta values [6, Theorem 1.1], we have the following theorem.

Theorem 4.1.5 (Brown)**.** *There is a non-canonical isomorphism $\mathcal{A} \to \mathcal{U}'$ of Hopf algebras that extends to an isomorphism*

$$\phi : \mathcal{H} \longrightarrow \mathcal{U} \tag{4.1.9}$$

of comodules for $\mathcal{A}$ and $\mathcal{U}'$, respectively, and which sends $\zeta^{\mathfrak{m}}(n)$ to f_n for all $n \geq 2$.

4.1.6 Depth filtration and depth-graded motivic MZVs

Definition 4.1.6 (depth filtration on the motivic MZV algebra)**.** Let $\mathcal{H}$ be the motivic MZV algebra $\bigoplus_{k\geq 0}\mathcal{H}_k$ as above. Let $\mathfrak{D}$ be the depth filtration on $\mathcal{H}$ defined by

$$\mathfrak{D}_0\mathcal{H} = \mathbb{Q} \subset \mathfrak{D}_1\mathcal{H} \subset \cdots \subset \mathfrak{D}_r\mathcal{H} := \langle \zeta^{\mathfrak{m}}(n_1,\ldots,n_j) : j \leq r\rangle_{\mathbb{Q}} \subset \cdots . \tag{4.1.10}$$

The motivic MZV algebra also becomes a filtered algebra under this depth filtration $\mathfrak{D}$, as in the case of the MZV algebra $\mathcal{Z}$ in Definition 3.1.2.

Definition 4.1.7 (depth-graded motivic MZV)**.** Let $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k$ be the $\mathbb{Q}$-vector space that is the weight k and depth r part of the bigraded $\mathbb{Q}$-algebra $\mathrm{gr}^{\mathfrak{D}}\mathcal{H} = \bigoplus_{k,r}\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k$. The depth-graded motivic MZV

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

is given by the class of $\zeta^{\mathfrak{m}}(n_1,\ldots,n_r)$ modulo elements of lower depth.

4.2 Motivic Broadhurst-Kreimer conjecture

In this section, we will state the motivic version of the Broadhurst-Kreimer conjecture [4, Conjecture 1] and its totally odd analogue [4, Conjecture 5].

Conjecture 4.2.1 (Motivic Broadhurst-Kreimer conjecture)**.** *The generating series of the dimensions of the spaces* $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k$ *is given by*

$$\sum_{k,r\geq 0}\dim_{\mathbb{Q}}(\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k)x^k y^r = \frac{1+\mathbb{E}(x)y}{1-\mathbb{O}(x)y+\mathbb{S}(x)y^2-\mathbb{S}(x)y^4}, \tag{4.2.1}$$

where $\mathbb{E}(x)$, $\mathbb{O}(x)$, $\mathbb{S}(x)$ *are defined as in Conjecture 3.1.6.*

We call $\zeta_{\mathfrak{D}}^{\mathfrak{m}}(n_1,\ldots,n_r)$ a totally odd motivic MZV when all n_i are odd and at least 3. The $\mathbb{Q}$-vector subspace of $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k$ spanned by all totally odd motivic MZVs of weight k and depth r is denoted by $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k^{\mathrm{odd}}$. As a convention, we set $\mathrm{gr}_0^{\mathfrak{D}}\mathcal{H}_0^{\mathrm{odd}}=\mathbb{Q}$. Now we have the following motivic version of the totally odd Broadhurst-Kreimer conjecture.

Conjecture 4.2.2 (Motivic totally odd Broadhurst-Kreimer conjecture)**.** *The generating series of the dimensions of the spaces* $\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k^{\mathrm{odd}}$ *is given by*

$$\sum_{k,r\geq 0}\dim_{\mathbb{Q}}(\mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}_k^{\mathrm{odd}})x^k y^r=\frac{1}{1-\mathbb{O}(x)y+\mathbb{S}(x)y^2}, \tag{4.2.2}$$

where $\mathbb{E}(x)$, $\mathbb{O}(x)$, $\mathbb{S}(x)$ *are defined as in Conjecture 3.1.6.*

Example 4.2.3. We will give the generating series for depth $2,3,4$ predicted by Conjecture 4.2.1 and Conjecture 4.2.2.

- $r=2$:

$$\begin{aligned}\sum_{k\geq 0}\dim_{\mathbb{Q}}(\mathrm{gr}_2^{\mathfrak{D}}\mathcal{H}_k)x^k &= \mathbb{O}^2(x)-\mathbb{S}(x)+(x^{\mathrm{odd}}\text{-terms})\\ \sum_{k\geq 0}\dim_{\mathbb{Q}}(\mathrm{gr}_2^{\mathfrak{D}}\mathcal{H}_k^{\mathrm{odd}})x^k &= \mathbb{O}^2(x)-\mathbb{S}(x)\end{aligned}$$

- $r=3$:

$$\begin{aligned}\sum_{k\geq 0}\dim_{\mathbb{Q}}(\mathrm{gr}_3^{\mathfrak{D}}\mathcal{H}_k)x^k &= \mathbb{O}^3(x)-2\mathbb{O}(x)\mathbb{S}(x)+(x^{\mathrm{even}}\text{-terms})\\ \sum_{k\geq 0}\dim_{\mathbb{Q}}(\mathrm{gr}_3^{\mathfrak{D}}\mathcal{H}_k^{\mathrm{odd}})x^k &= \mathbb{O}^3(x)-2\mathbb{O}(x)\mathbb{S}(x)\end{aligned}$$

- $r = 4$:

$$\sum_{k\geq 0} \dim_{\mathbb{Q}}(\mathrm{gr}_4^{\mathfrak{D}}\mathcal{H}_k)x^k = \mathbb{O}^4(x) - 3\mathbb{O}(x)^2\mathbb{S}(x) + \mathbb{S}^2(x) + \mathbb{S}(x) + (x^{\mathrm{odd}}\text{-terms})$$
$$\sum_{k\geq 0} \dim_{\mathbb{Q}}(\mathrm{gr}_4^{\mathfrak{D}}\mathcal{H}_k^{\mathrm{odd}})x^k = \mathbb{O}^4(x) - 3\mathbb{O}(x)^2\mathbb{S}(x) + \mathbb{S}^2(x)$$

When $r = 2, 3$, Conjecture 4.2.2 is known from the work of Zagier [39] and Goncharov [17]. The terms in the parentheses are known explicitly, but we will not discuss them here. Notice that there is an extra $\mathbb{S}(x)$ in the depth 4 cases, which conjecturally arises from the depth 4 elements $\bar{\mathfrak{e}}$ or $\mathfrak{c}$ discussed in Sections 7.4 and 7.5.

4.3 Operator D_p

In this section, we will introduce Brown's operator D_p for odd $p \geq 3$. Then we will use it to compute the image of $\phi : \mathcal{H} \to \mathcal{U}$ for the depth 2 motivic MZVs. At the end, we will construct a matrix whose right annihilator gives us the linear relations between depth 2 motivic MZVs modulo motivic single zeta values.

Before introducing the operator D_p, let us recall an infinitesimal version of the coaction $\Delta : \mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$ introduced by Brown [6, Definition 3.1]. Let $\mathcal{L} := \mathcal{A}_{>0}/(\mathcal{A}_{>0})^2$ be the tangent space of the Hopf algebra $\mathcal{A}$, and let $\pi_p : \mathcal{A}_{>0} \to \mathcal{L}_p$ be the natural projection taking the graded part of weight p of the graded vector space $\mathcal{L} = \bigoplus_{p>0} \mathcal{L}_p$.

Definition 4.3.1 (The Brown operator)**.** We define a linear map $D_p : \mathcal{H} \to \mathcal{L}_p \otimes_{\mathbb{Q}} \mathcal{H}$ for all odd integers $p > 1$ as the following composition:

$$D_p : \mathcal{H} \xrightarrow{\Delta - 1\otimes \mathrm{id}} \mathcal{A}_{>0} \otimes_{\mathbb{Q}} \mathcal{H} \xrightarrow{\pi_p \otimes \mathrm{id}} \mathcal{L}_p \otimes_{\mathbb{Q}} \mathcal{H}.$$

One can easily check that the map D_p is a derivation. From Theorem 4.1.4, we find that the formula ([4, Proposition 3.2]) for the map D_p is given by

$$D_p I^{\mathfrak{m}}(a_0; a_1, \dots, a_n; a_{n+1}) = \sum_{m=0}^{n-p} \pi_m(I^{\mathfrak{a}}(a_m; a_{m+1}, \dots, a_{m+p}; a_{m+p+1})) \otimes I^{\mathfrak{m}}(a_0; a_1, \dots, a_m, a_{m+p+1}, \dots, a_n; a_{n+1}). \tag{4.3.1}$$

Using Brown's notation in [4], we call the sequence $(a_m; a_{m+1}, \dots, a_{m+p}; a_{m+p+1})$ appearing in the first factor a subsequence of length p and the sequence $(a_0; a_1, \dots, a_m, a_{m+p+1}, \dots, a_n; a_{n+1})$ in the second factor the corresponding quotient sequence. The depth of a sequence $(a_0; a_1, \dots, a_n; a_{n+1})$ with $a_0 \neq a_{n+1}$ is defined to be the number of 1's in $a_1, \dots, a_n$, while the depth of a sequence $(a_0; a_1, \dots, a_n; a_{n+1})$ with $a_0 = a_{n+1}$ is defined to be 0.

For later use, we compute Brown's operator explicitly in depth 2. We use the same notation as in [35]. Define the integer $b^m_{n,n'}$ $(n, n', m \in \mathbb{Z})$ by

$$b^m_{n,n'} = (-1)^n \binom{m-1}{n-1} + (-1)^{n'-m} \binom{m-1}{n'-1},$$

where $\binom{n}{m} = 0$ for each $m < 0$. Define the integer $e\binom{m_1, m_2}{n_1, n_2}$ $(n_1, n_2, m_1, m_2 \in \mathbb{Z})$ by

$$e\binom{m_1, m_2}{n_1, n_2} = \delta\binom{m_1, m_2}{n_1, n_2} + b^{m_1}_{n_1, n_2} \in \mathbb{Z}, \tag{4.3.2}$$

where $\delta\binom{v}{w}$ is the Kronecker delta symbol for vectors v and w defined by

$$\delta\binom{v}{w} = \begin{cases} 1 & \text{if } v = w; \\ 0 & \text{otherwise .} \end{cases}$$

Let us denote by ξ_p the image of $\zeta^{\mathfrak{m}}(p)$ in the space $\mathcal{L}$ and by $\mathfrak{D}_r\mathcal{H}$ the $\mathbb{Q}$-vector space spanned by all motivic multiple zeta values of depth $\leq r$ as in Definition 4.1.6. Then we have the following proposition.

Proposition 4.3.2. *For any integers $n_1, n_2 \geq 1$ with $k = n_1 + n_2$ and odd $p \geq 3$, the element*

$$D_p\big(\zeta^{\mathfrak{m}}(n_1, n_2)\big) - e\tbinom{p,k-p}{n_1,n_2}\xi_p \otimes \zeta^{\mathfrak{m}}(k-p)$$

lies in $\mathcal{L}_p \otimes \mathfrak{D}_0\mathcal{H}_{k-p}$, where $\mathfrak{D}_r\mathcal{H}_k = \mathfrak{D}_r\mathcal{H} \cap \mathcal{H}_k$.

Proof of Proposition 4.3.2. We apply D_p, with odd $p \geq 3$, to the element

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

Every subsequence of depth ≥ 2 gives rise to a quotient sequence of depth 0, so the corresponding term in the image of D_p lies in $\mathcal{L}_p \otimes \mathfrak{D}_0\mathcal{H}_{k-p}$. So we only need to consider the case when the subsequence is of depth 1. Every subsequence of depth 1 and length p must be one of the following two forms:

$$\text{(a)} \qquad (0; \underbrace{0, \ldots, 0}_{i}, 1, \underbrace{0, \ldots, 0}_{j}; 1),$$
$$\text{(b)} \qquad (1; \underbrace{0, \ldots, 0}_{i}, 1, \underbrace{0, \ldots, 0}_{j}; 0),$$

where $i + j + 1 = p$ with $i, j \geq 0$. By $\mathbf{I_3}$ in Section 4.1.3, the case (b) can be computed from case (a) with an extra minus sign. For the case (a), by $\mathbf{I_0}$, $\mathbf{I_2}$ and $\mathbf{I_3}$, we have

$$\begin{aligned} & I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0}_{i}, 1, \underbrace{0, \ldots, 0}_{j}; 1) \\ \overset{\mathbf{I_2}}{=} & \sum_{\substack{r+s=i+j \\ r,s \geq 0}} (-1)^{r-j} \binom{r}{j} I^{\mathfrak{m}}(0; 1, \underbrace{0, \ldots, 0}_{r}; 1) I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0}_{s}; 1) \\ \overset{\mathbf{I_0},\mathbf{I_3}}{=} & (-1)^i \binom{i+j}{j} \zeta^{\mathfrak{m}}(i+j+1). \end{aligned}$$

Thus, every subsequence of depth 1 and length p produces an element in $\mathbb{Q}\xi_p \otimes \mathfrak{D}_1\mathcal{H}_{k-p}$. Summing up the two terms corresponding to cases (a) and (b) and the possible third term appearing exactly when $p = n_1$ in the image of $D_p I^{\mathfrak{m}}(0; 1, \underbrace{0, \ldots, 0}_{n_1-1}, 1, \underbrace{0, \ldots, 0}_{n_2-1}; 1)$, one obtains

$$\begin{aligned}
& \delta\tbinom{n_1}{p}\pi_p(I^{\mathfrak{m}}(0; 1, \underbrace{0, \ldots, 0}_{n_1-1}; 1)) \otimes I^{\mathfrak{m}}(0; 1, \underbrace{0, \ldots, 0}_{n_2-1}; 1) \\
& + \pi_p(I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0}_{p-n_2}, 1, \underbrace{0, \ldots, 0}_{n_2-1}; 1)) \otimes I^{\mathfrak{m}}(0; 1, \underbrace{0, \ldots, 0}_{k-p-1}; 1) \\
& + \pi_p(I^{\mathfrak{m}}(1; \underbrace{0, \ldots, 0}_{n_1-1}, 1, \underbrace{0, \ldots, 0}_{p-n_1}; 0)) \otimes I^{\mathfrak{m}}(0; 1, \underbrace{0, \ldots, 0}_{k-p-1}; 1) \\
= \; & \delta\tbinom{n_1}{p}\xi_{n_1} \otimes \zeta^{\mathfrak{m}}(n_2) \\
& + (-1)^{n_2-p}\tbinom{p-1}{n_2-1}\xi_p \otimes \zeta^{\mathfrak{m}}(k-p) \\
& + (-1)^{n_1}\tbinom{p-1}{n_1-1}\xi_p \otimes \zeta^{\mathfrak{m}}(k-p) \\
= \; & e\tbinom{p,k-p}{n_1,n_2}\xi_p \otimes \zeta^{\mathfrak{m}}(k-p),
\end{aligned}$$

which completes the proof. □

By composing with the isomorphism $\phi : \mathcal{H} \to \mathcal{U}$, we have the following corollary.

Corollary 4.3.3. *For any integers $k, n_1, n_2 \geq 1$ with $k = n_1 + n_2$, the image of $\zeta^{\mathfrak{m}}(n_1, n_2)$ under the isomorphism ϕ can be written in the form*

$$\phi(\zeta^{\mathfrak{m}}(n_1, n_2)) = \sum_{\substack{m_1+m_2=k \\ m_1 \geq 3:\text{odd} \\ m_2 \geq 2}} e\tbinom{m_1,m_2}{n_1,n_2} f_{m_1} f_{m_2} + a f_k$$

for some $a \in \mathbb{Q}$.

Proof of Corollary 4.3.3. We recall the infinitesimal version of the coaction $\Delta^{\bullet}$: $\mathcal{U} \to \mathcal{U}' \otimes \mathcal{U}$ (see [6, (2.25)] and [6, Lemma 2.4]). Set $L := \mathcal{U}'_{>0}/\left(\mathcal{U}'_{>0}\right)^2$, which is a graded vector space $L = \bigoplus_{p>0} L_p$. Let $\pi'_p : \mathcal{U}'_{>0} \to L_p$ be the projection. For each odd $p \geq 3$, let us define $D^\bullet_p$ by the composite map

$$D^\bullet_p : \mathcal{U} \xrightarrow{\Delta^\bullet - 1 \otimes \mathrm{id}} \mathcal{U}'_{>0} \otimes \mathcal{U} \xrightarrow{\pi'_p \otimes \mathrm{id}} L_p \otimes \mathcal{U}.$$

By Theorem 4.1.5, the following diagram commutes:

$$\begin{array}{ccc} \mathcal{H} & \xrightarrow{D_p} & \mathcal{L}_p \otimes \mathcal{H} \\ \downarrow{\scriptstyle \phi} & & \downarrow{\scriptstyle \overline{\phi} \otimes \phi} \\ \mathcal{U} & \xrightarrow{D^\bullet_p} & L_p \otimes \mathcal{U} \end{array}$$

where $\overline{\phi}$ is the isomorphism $\overline{\phi} : \mathcal{L} \to L$ induced by ϕ, which sends ξ_p to $\overline{f}_p := \pi'_p(f_p)$. This commutative diagram says that the D_p and $D^\bullet_p$ defined for $\mathcal{H}$ and $\mathcal{U}$ are compatible with the isomorphism $\phi : \mathcal{H} \to \mathcal{U}$.

Then by Proposition 4.3.2, we have

$$\begin{aligned} \sum_{\substack{1<p<k \\ p:\text{odd}}} D^\bullet_p \circ \phi(\zeta^{\mathfrak{m}}(n_1, n_2)) &= \sum_{\substack{1<p<k \\ p:\text{odd}}} (\overline{\phi} \otimes \phi) \circ D_p(\zeta^{\mathfrak{m}}(n_1, n_2)) \\ &= \sum_{\substack{1<p<k \\ p:\text{odd}}} e\binom{p,k-p}{n_1,n_2} \overline{f}_p \otimes f_{k-p}, \end{aligned} \tag{4.3.3}$$

where we take $f_1 = 0$ as a convention. On the other hand, we also have

$$\sum_{\substack{1<p<k \\ p:\text{odd}}} D^\bullet_p \Bigg(\sum_{\substack{m_1+m_2=k \\ m_1 \geq 3:\text{odd} \\ m_2 \geq 2}} e\binom{m_1,m_2}{n_1,n_2} f_{m_1} f_{m_2} \Bigg) = \sum_{\substack{m_1+m_2=k \\ m_1 \geq 3:\text{odd} \\ m_2 \geq 2}} e\binom{m_1,m_2}{n_1,n_2} \overline{f}_{m_1} \otimes f_{m_2}. \tag{4.3.4}$$

Taking the difference between (4.3.3) and (4.3.4), we have

$$\phi(\zeta^{\mathfrak{m}}(n_1, n_2)) - \sum_{\substack{m_1+m_2=k \\ m_1 \geq 3:\text{odd} \\ m_2 \geq 2}} e\binom{m_1,m_2}{n_1,n_2} f_{m_1} f_{m_2} \in \ker \sum_{\substack{1<p<k \\ p:\text{odd}}} D^\bullet_p,$$

Then, by [6, Lemma 2.7], which says that

$$\ker \sum_{\substack{1<p<k \\ p:\text{odd}}} D_p^{\bullet}\big|_{\mathcal{U}_k} = \mathbb{Q} f_k,$$

the statement follows. □

Using the above corollary, we make the following definition.

Definition 4.3.4 (Matrix $\mathcal{C}_k^I$)**.** For any positive integer k and any double index set $I \subseteq \{(n_1, n_2) \mid n_1 \geq 1, n_2 \geq 2, n_1 + n_2 = k\}$, define

$$\mathcal{C}_k^I = \left(e\binom{m_1, m_2}{n_1, n_2} \right)_{\substack{m_1 \geq 3:\text{odd} \\ m_2 \geq 2 \\ (n_1,n_2) \in I}}. \tag{4.3.5}$$

As a corollary of Corollary 4.3.3, we have the following result.

Corollary 4.3.5. *Every element in the right annihilator of $\mathcal{C}_k^I$ gives a linear relation between motivic double zeta values of weight k with indices in the set I, modulo motivic single zeta values.*

Proof of Corollary 4.3.5. For any element $v = (v_{(n_1,n_2)})^T_{(n_1,n_2)\in I} \in \ker((\mathcal{C}_k^I)^T)$, we have

$$\sum_{(n_1,n_2)\in I} v_{(n_1,n_2)} e\binom{m_1, m_2}{n_1, n_2} = 0 \text{ for all } (m_1, m_2).$$

Then we have

$$\begin{aligned} &\phi\Bigg(\sum_{(n_1,n_2)\in I} v_{(n_1,n_2)} \zeta^{\mathfrak{m}}(n_1, n_2) \Bigg) \\ = &\sum_{(n_1,n_2)\in I} v_{(n_1,n_2)} \phi\big(\zeta^{\mathfrak{m}}(n_1, n_2)\big) \end{aligned}$$

$$
\begin{aligned}
&= \sum_{(n_1,n_2)\in I} v_{(n_1,n_2)} \Bigg(\sum_{\substack{m_1+m_2=k\\ m_1\geq 3:\text{odd}\\ m_2\geq 2}} e\binom{m_1,m_2}{n_1,n_2} f_{m_1} f_{m_2} + a_{(n_1,n_2)} f_k \Bigg) \\
&= \sum_{(n_1,n_2)\in I} v_{(n_1,n_2)} a_{(n_1,n_2)} f_k \\
&= \phi\Bigg(\sum_{(n_1,n_2)\in I} v_{(n_1,n_2)} a_{(n_1,n_2)} \zeta^{\mathfrak{m}}(k) \Bigg).
\end{aligned}
$$

Since $\phi : \mathcal{H} \to \mathcal{U}$ is an isomorphism, we have shown the statement. □

4.4 Classical results in the motivic setting

4.4.1 Gangl-Kaneko-Zagier's result in the motivic setting

In this section, we will reformulate Theorem 3.2.1 in the motivic setting. In [1, Proposition 3.2], for each even $k \geq 6$, Baumard and Schneps defined a $\frac{k-4}{2} \times \frac{k-4}{2}$ matrix A_k with entries

$$
(A_k)_{i,j} = \binom{2i}{2j} - \binom{2i}{k-2-2j} + \delta\binom{\frac{k-2}{2}}{i+j}
$$

Remark. This is actually the transpose of the matrix considered in [1, Proposition 3.2]. Here we use this definition in order to compare with the $\mathcal{C}_k^I$ defined above.

We have the following result for this matrix A_k from [1, Proposition 3.2].

Proposition 4.4.1 (Baumard-Schneps)**.** *For all even $k \geq 12$, the space $\mathbf{W}_k^{-,0}$ of weight k restricted period polynomials is in bijection with the kernel of the matrix A_k.*

Baumard and Schneps constructed an isomorphism of $\mathbb{Q}$-vector spaces from $\ker(A_k)$ to $\ker(A_k^T)$ in [1, Proposition 3.4].

Proposition 4.4.2 (Baumard-Schneps)**.** *Let* $k \geq 12$ *be even, and suppose that* $(a_1, a_2, \ldots, -a_2, -a_1) \in \ker A_k$*. Set*

$$P(X,Y) = \sum_{i=1}^{\lfloor \frac{k-4}{4} \rfloor} a_i (X^{2i}Y^{k-2-2i} - X^{k-2-2i}Y^{2i}),$$

and define the coefficient $q_{r,k-r}$ *for* $1 \leq r \leq k-3$ *by*

$$P(X+Y,Y) = \sum_{r=1}^{k-3} \binom{k-2}{r-1} q_{r,k-r} X^{r-1}Y^{k-r-1}.$$

Then the vector $(q_{3,k-3}, \ldots, q_{k-3,3})$ *(with odd indices) lies in the kernel of* A_k^T*, and in fact the kernel of* A_k^T *consists of exactly these vectors.*

Baumard and Schneps then recovered Theorem 3.2.1 as the following corollary ([1, Corollary of Proposition 3.4]).

Corollary 4.4.3. *Let* $k \geq 12$ *be an even integer, let* $P(X,Y) \in \mathbf{W}_k^{-,0}$ *be a restricted even period polynomial of weight* k*, and write*

$$P(X+Y,Y) = \sum_{r=1}^{k-3} \binom{k-2}{r-1} q_{r,k-r} X^{r-1}Y^{k-r-1}.$$

Then the linear combination

$$\sum_{\substack{r=3 \\ r:\text{odd}}}^{k-3} q_{r,k-r} Z_{r,k-r}$$

is equal to a scalar multiple of Z_k *in the formal double zeta space* $\mathbf{D}_k$*.*

Now let us look at the matrix A_k in detail. Recall the matrix $\mathcal{C}_k^I$ of Definition 4.3.4. Suppose that $k \geq 6$ is an even integer, and let $I = \{(k-3,3), (k-5,5), \ldots, (3, k-3)\}$. Then we have

$$(\mathcal{C}_k^I)_{i,j} \quad = \quad (\mathcal{C}_k^I)_{\substack{(2i+1,k-2i-1) \\ (k-2j-1,2j+1)}}$$

$$
\begin{aligned}
&= e\tbinom{2i+1,k-2i-1}{k-2j-1,2j+1} \\
&= \delta\tbinom{2i+1,k-2i-1}{k-2j-1,2j+1} + b^{2i+1}_{k-2j-1,2j+1} \\
&= \delta\tbinom{2i+1,k-2i-1}{k-2j-1,2j+1} + (-1)^{k-2j-1}\binom{2i}{k-2-2j} + (-1)^{2j-2i}\binom{2i}{2j} \\
&= \delta\binom{\frac{k-2}{2}}{i+j} - \binom{2i}{k-2-2j} + \binom{2i}{2j} \\
&= (A_k)_{i,j}
\end{aligned}
$$

This shows that the matrix A_k is nothing but the matrix $\mathcal{C}_k^I$ with $I = \{(k-3,3),(k-5,5),\ldots,(3,k-3)\}$. Hence by Corollary 4.3.5, we have the following motivic version of Theorem 3.2.1 of Gangl-Kaneko-Zagier.

Corollary 4.4.4 (Motivic version of the GKZ theorem)**.** *Let $k \geq 12$ be an even integer, let $P(X,Y) \in \mathbf{W}_k^{-,0}$ be a restricted even period polynomial of weight k, and write*

$$P(X+Y,Y) = \sum_{r=1}^{k-3} \binom{k-2}{r-1} q_{r,k-r} X^{r-1} Y^{k-r-1}.$$

Then the linear combination

$$\sum_{\substack{r=3 \\ r:\text{odd}}}^{k-3} q_{r,k-r}\zeta^{\mathfrak{m}}(k-r,r)$$

is equal to a scalar multiple of $\zeta^{\mathfrak{m}}(k)$ in the motivic MZV algebra $\mathcal{H}$.

4.4.2 The decomposition formula in the motivic setting

In this section, we will state the motivic version of Proposition 3.3.1. First of all, let us look at Euler's decomposition relations (3.3.1) modulo $\mathbb{Q}\zeta(k)$. For any odd integer k, we have

$$\zeta(m,n) \equiv (-1)^m \sum_{s=1}^{\frac{k-3}{2}} \left[\binom{k-2s-1}{m-1} + \binom{k-2s-1}{n-1} - \delta_{n,2s} \right] \zeta(2s)\zeta(k-2s) \tag{4.4.1}$$

Using the notation in [36], we can use the above decomposition formula (4.4.1) to define two square $\mathbb{Z}$-matrices $\mathcal{A}_k$ and $\mathcal{A}'_k$ corresponding to the two parities (even, odd) and (odd, even).

$$(\zeta(2)\zeta(k-2), \zeta(4)\zeta(k-4), \ldots, \zeta(k-3)\zeta(3))\mathcal{A}_k \tag{4.4.2}$$
$$\equiv (\zeta(2,k-2), \zeta(4,k-4), \ldots, \zeta(k-3,3)) \pmod{\zeta(k)}$$
$$(\zeta(2)\zeta(k-2), \zeta(4)\zeta(k-4), \ldots, \zeta(k-3)\zeta(3))\mathcal{A}'_k \tag{4.4.3}$$
$$\equiv (\zeta(3,k-3), \zeta(5,k-5), \ldots, \zeta(k-2,2)) \pmod{\zeta(k)}$$

Later we set $\mathcal{A} := \mathcal{A}_k$ if k is clear from the context. By the same computation as in the last section, we have

$$\mathcal{A}_k = \mathcal{C}_k^{I_1} \qquad \text{with } I_1 = \{(2,k-2),(4,k-4),\ldots,(k-3,3)\},$$
$$\mathcal{A}'_k = \mathcal{C}_k^{I_2} \qquad \text{with } I_2 = \{(3,k-3),(5,k-5),\ldots,(k-2,2)\}.$$

Since

$$\phi(\zeta^{\mathfrak{m}}(2i+1)\zeta^{\mathfrak{m}}(2j)) = f_{2i+1}f_{2j},$$

Corollary 4.3.3 implies that Euler's decomposition formula also holds in the motivic setting, i.e., we have

Proposition 4.4.5 (Motivic version of Euler's decomposition formula)**.** *Let $k \geq 5$ be an odd integer. The motivic double zeta value $\zeta^{\mathfrak{m}}(m,n)$ $(m \geq 1, n \geq 2)$ of weight*

$m+n=k$ can be written as

$$\begin{aligned}\zeta^{\mathfrak{m}}(m,n) &= (-1)^m \sum_{s=1}^{\frac{k-3}{2}} \left[\binom{k-2s-1}{m-1} + \binom{k-2s-1}{n-1} - \delta_{n,2s}\right] \zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s) \\ &\quad -\frac{1}{2}(-1)^m \left[\binom{k-1}{m-1} + \binom{k-1}{n-1} + (-1)^m\right]\zeta^{\mathfrak{m}}(k) \qquad (4.4.4)\end{aligned}$$

We separate out the following two cases corresponding to two different parities.

$$(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2), \zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4), \ldots, \zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3))\mathcal{A}_k \qquad (4.4.5)$$

$$\equiv (\zeta^{\mathfrak{m}}(2,k-2), \zeta^{\mathfrak{m}}(4,k-4), \ldots, \zeta^{\mathfrak{m}}(k-3,3)) \pmod{\zeta^{\mathfrak{m}}(k)}$$

$$(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2), \zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4), \ldots, \zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3))\mathcal{A}'_k \qquad (4.4.6)$$

$$\equiv (\zeta^{\mathfrak{m}}(3,k-3), \zeta^{\mathfrak{m}}(5,k-5), \ldots, \zeta^{\mathfrak{m}}(k-2,2)) \pmod{\zeta^{\mathfrak{m}}(k)}$$

The properties of $\mathcal{A}_k$ and $\mathcal{A}'_k$ will be discussed in detail in the next two chapters.

CHAPTER 5

Double Zeta Values of Parity (even, odd)

In this chapter, we will study the (motivic) double zeta values of parity (even, odd). We first look at the matrix $\mathcal{A} := \mathcal{A}_k$ defined in the last chapter. We will prove a result conjectured by Zagier on the explicit expression for the inverse matrix $\mathcal{A}^{-1}$. As corollaries, we obtain a family of Bernoulli number identities, and we also obtain two families of relations between (motivic) double zeta values of odd weight, which we call the standard relations. The results in Sections 5.1–5.3 can be found in [26]. Throughout this chapter, $k = 2K + 1$ will be an odd integer at least 5, and B_n is the nth Bernoulli number.

5.1 Inverse matrix theorem

In [36, Lemma 3], Zagier proved the following result.

Lemma 5.1.1 (Zagier)**.** *The determinant of the matrix $\mathcal{A}$ is nonzero.*

Zagier conjectured in [36, Page 993] the following two explicit formulas for the inverse matrix $\mathcal{A}^{-1}$. We will prove this conjecture in the next section, and we state it as a theorem here.

Theorem 5.1.2. *For $1 \leq s, r \leq K - 1$, we have*

$$\left(\mathcal{A}^{-1}\right)_{r,s} = \frac{-2}{2s-1} \sum_{n=0}^{k-2s} \binom{k-2r-1}{k-2s-n} \binom{n+2s-2}{n} B_n \tag{5.1.1}$$

$$= \frac{2}{2s-1}\sum_{n=0}^{k-2s}\binom{2r-1}{k-2s-n}\binom{n+2s-2}{n}B_n. \qquad (5.1.2)$$

In particular, the first and the last rows of $\mathcal{A}^{-1}$ consist of simple multiples of Bernoulli numbers, as the next corollary says.

Corollary 5.1.3. *For any s satisfying $1 \leq s \leq K-2$, we have*

$$\left(\mathcal{A}^{-1}\right)_{1,s} = -\frac{1}{2}\left(\mathcal{A}^{-1}\right)_{K-1,s} = 2\binom{2K-2}{2s-1}\frac{B_{2K-2s}}{2K-2s}. \qquad (5.1.3)$$

Also by using $\mathcal{A}^{-1}$, we can explicitly express the products $\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)$, $1 \leq s \leq K-1$ in terms of motivic double zeta values $\zeta^{\mathfrak{m}}(2r, k-2r)$, $1 \leq r \leq K-1$, as the next corollary says.

Corollary 5.1.4. *Modulo $\mathbb{Q}\zeta^{\mathfrak{m}}(k)$, the products $\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)$, $1 \leq s \leq K-1$, can be expressed in terms of motivic double zeta values $\zeta^{\mathfrak{m}}(2r, k-2r)$, $1 \leq r \leq K-1$ as follows*

$$\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s) \equiv \sum_{r=1}^{K-1}\left(\mathcal{A}^{-1}\right)_{r,s}\zeta^{\mathfrak{m}}(2r, k-2r) \pmod{\zeta^{\mathfrak{m}}(k)}, \qquad (5.1.4)$$

where $\left(\mathcal{A}^{-1}\right)_{r,s}$ is given by either (5.1.1) or (5.1.2).

5.2 Proof of the results

5.2.1 Proof of Theorem 5.1.2

In this section, we will define two 2-variable polynomials, and state a result about one of them. Later, in Lemma 5.2.5, we will see that the result also holds for the other one by proving that they are identical to each other.

Definition 5.2.1. For any $0 \leq i \leq k-2$, we define the following two polynomials

$$F_k^{(i)}(x,y) = \sum_{s=1}^{K-1} \left(\frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{i}{k-2s-n} \binom{n+2s-2}{n} B_n \right) x^{2K-2s} y^{2s-1}; \quad (5.2.1)$$

$$G_k^{(i)}(x,y) = \sum_{s=1}^{K-1} \left(\frac{-2}{2s-1} \sum_{n=0}^{k-2s} \binom{k-2-i}{k-2s-n} \binom{n+2s-2}{n} B_n \right) x^{2K-2s} y^{2s-1}. \quad (5.2.2)$$

Notice that the two polynomials correspond to the two expressions (5.1.1), (5.1.2) for $\mathcal{A}^{-1}$, and it is clear from the definition that we have

$$F_k^{(i)}(x,y) = -G_k^{(k-2-i)}(x,y).$$

The two polynomials $F_k^{(i)}(x,y)$ and $G_k^{(i)}(x,y)$ are closely related to the following polynomial.

Definition 5.2.2. For any $0 \leq i \leq k-2$, we define the following polynomial

$$R_k^{(i)}(x,y) = \frac{k-2-2i}{k-2} x^{k-2} + (-1)^{i-1} x^{k-2-i} y^i + (-1)^{i-1} x^i y^{k-2-i} + \frac{k-2-2i}{k-2} y^{k-2}. \quad (5.2.3)$$

The connection between $F_k^{(i)}(x,y)$, $G_k^{(i)}(x,y)$ and $R_k^{(i)}(x,y)$ can be stated as the following theorem, whose proof will be postponed to Section 5.2.2.

Theorem 5.2.3. *For any $0 \leq i \leq k-2$, we have*

$$F_k^{(i)}(x+y,x) + F_k^{(i)}(x+y,y) = R_k^{(i)}(x,y) \quad (5.2.4)$$

$$G_k^{(i)}(x+y,x) + G_k^{(i)}(x+y,y) = R_k^{(i)}(x,y) \quad (5.2.5)$$

Assuming Theorem 5.2.3, we are able to prove Theorem 5.1.2 now.

Proof of Theorem 5.1.2. According to the definition of the matrix $\mathcal{A}$, we have

$$\mathcal{A}_{s,r} = \binom{2K-2s}{2r-1} + \binom{2K-2s}{2K-2r}.$$

For the vector $v = (v_1, v_2, \ldots, v_{K-1})$, define its associated polynomial to be $V(x,y) = \sum_{s=1}^{K-1} v_s x^{2K-2s} y^{2s-1}$. We also call this vector v the associated vector of $V(x,y)$. Assume that $v\mathcal{A} = w := (w_1, w_2, \ldots, w_{K-1})$. Then the associated polynomial of w is

$$\begin{aligned} W(x,y) &:= \sum_{j=1}^{K-1} w_j x^{2j-1} y^{2K-2j} \\ &= \text{sum of } x^{2j-1}y^{2K-2j}\text{-terms in } V(x+y,x) + V(x+y,y), \end{aligned}$$

where $V(x+y,x)$ and $V(x+y,y)$ give us the terms $\binom{2K-2s}{2r-1}$ and $\binom{2K-2s}{2K-2r}$ in $\mathcal{A}_{s,r}$, respectively.

According to Theorem 5.2.3, for $1 \le i \le K-1$, we have

$$\begin{aligned} & \text{sum of } x^{2j-1}y^{2K-2j}\text{-terms in } F_k^{(2i-1)}(x+y,x) + F_k^{(2i-1)}(x+y,y) \\ = \; & \text{sum of } x^{2j-1}y^{2K-2j}\text{-terms in } R_k^{(2i-1)}(x,y) \\ = \; & x^{2i-1}y^{2K-2i}. \end{aligned}$$

Therefore, for the matrix with ith row coming from the associated vector of $F_k^{(2i-1)}(x,y)$, its product with $\mathcal{A}$ gives us the identity matrix, i.e., we have

$$\left(\mathcal{A}^{-1}\right)_{r,s} = \frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{2r-1}{k-2s-n} \binom{n+2s-2}{n} B_n \qquad (1 \le s, r \le K-1).$$

By considering G_k instead of F_k, we obtain (5.1.2). $\square$

As a corollary, the first and the last rows of $\mathcal{A}^{-1}$ can be reduced to simple multiples of Bernoulli numbers.

Proof of Corollary 5.1.3. When $r = 1$ and $1 \leq s \leq K-2$, we have

$$\begin{aligned}
\left(\mathcal{A}^{-1}\right)_{1,s} &\overset{(5.1.2)}{=} \frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{1}{k-2s-n} \binom{n+2s-2}{n} B_n \\
&= \frac{2}{2s-1} \binom{k-2s-1+2s-2}{k-2s-1} B_{k-2s-1} \\
&= \frac{2}{2s-1} \binom{2K-2}{2s-2} B_{2K-2s} \\
&= 2\binom{2K-2}{2s-1} \frac{B_{2K-2s}}{2K-2s}.
\end{aligned}$$

When $r = K-1$ and $1 \leq s \leq K-2$, we have

$$\begin{aligned}
\left(\mathcal{A}^{-1}\right)_{K-1,s} &\overset{(5.1.1)}{=} \frac{-2}{2s-1} \sum_{n=0}^{k-2s} \binom{2}{k-2s-n} \binom{n+2s-2}{n} B_n \\
&= \frac{-2}{2s-1} \binom{2}{1} \binom{k-2s-1+2s-2}{k-2s-1} B_{k-2s-1} \\
&= \frac{-4}{2s-1} \binom{2K-2}{2s-2} B_{2K-2s} \\
&= -4\binom{2K-2}{2s-1} \frac{B_{2K-2s}}{2K-2s}.
\end{aligned}$$

□

Corollary 5.1.4 is by Proposition 4.4.5 just a reformulation of the fact that $\mathcal{A}\mathcal{A}^{-1} = I_{K-1}$.

5.2.2 Proof of Theorem 5.2.3

In this section, we will state four lemmas and use them to prove Theorem 5.2.3. The proofs of those lemmas will be provided in Section 5.2.3.

The first lemma tells us that the second derivatives in y of $F_k^{(i)}(x,y)$ and $G_k^{(i)}(x,y)$ can be expressed as linear combinations of $F_{k-2}^{(j)}(x,y)$ and $G_{k-2}^{(j)}(x,y)$ for certain values of j.

Lemma 5.2.4. *For any* $0 \leq i \leq k-2$*, we have*

$$\frac{\partial^2}{\partial y^2} F_k^{(i)} = (k-2-i)(k-3-i)F_{k-2}^{(i)} - 2i(k-2-i)G_{k-2}^{(k-3-i)} + i(i-1)F_{k-2}^{(i-2)}, \tag{5.2.6}$$

$$\frac{\partial^2}{\partial y^2} G_k^{(i)} = (k-2-i)(k-3-i)G_{k-2}^{(i)} - 2i(k-2-i)F_{k-2}^{(k-3-i)} + i(i-1)G_{k-2}^{(i-2)}. \tag{5.2.7}$$

Although we do not have the definitions of $F_{k-2}^{(i)}$ and $G_{k-2}^{(i)}$ for $i = -1$ or -2, we can see from the above expressions that the coefficients before them would be 0.

The next lemma says that $F_k^{(i)}(x, y)$ and $G_k^{(i)}(x, y)$ are actually identical to each other.

Lemma 5.2.5. *For any* $0 \leq i \leq k-2$*, we have*

$$F_k^{(i)}(x, y) = G_k^{(i)}(x, y) \tag{5.2.8}$$

Later, in Section 5.3, we will show that the above lemma can be extended to a more general setting, which will give us more Bernoulli number identities. Not only do $F_k^{(i)}$ and $G_k^{(i)}$ have nice properties for the second derivatives in y, but $R_k^{(i)}$ also has one, as the next lemma claims.

Lemma 5.2.6. *For any* $0 \leq i \leq k-2$*, we have*

$$\begin{aligned} \frac{\partial^2}{\partial y^2}\left(R_k^{(i)}(x-y, y)\right) \quad = \quad & (k-2-i)(k-3-i)R_{k-2}^{(i)}(x-y, y) \\ & -2i(k-2-i)R_{k-2}^{(k-3-i)}(x-y, y) \\ & +i(i-1)R_{k-2}^{(i-2)}(x-y, y) \end{aligned} \tag{5.2.9}$$

The next lemma gives a tool to compute the coefficient of $x^{k-3}y$ in $F_k^{(i)}(x, x-y)$.

Lemma 5.2.7. *For any positive integers k and i satisfying $k \geq 4$ and $1 \leq i \leq k-3$, we have*

$$A_k^{(i)} := \sum_{s=1}^{\lfloor \frac{k}{2} \rfloor} \frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{i}{k-2s-n} \binom{n+2s-2}{n} B_n = 0. \tag{5.2.10}$$

Moreover, under the same assumption on k, we have

$$A_k^{(0)} = (-1)^k. \tag{5.2.11}$$

Now we can use the above four lemmas to prove Theorem 5.2.3.

Proof of Theorem 5.2.3. We need only prove the following identity, which is obtained from (5.2.4) by the change-of-variables $x \mapsto x-y$ and $y \mapsto y$:

$$F_k^{(i)}(x, x-y) + F_k^{(i)}(x, y) = R_k^{(i)}(x-y, y). \tag{5.2.12}$$

When $i = 0$, we have $F_k^{(0)}(x, y) = R_k^{(0)}(x, y) = 0$ by definition and the properties that $\binom{0}{n} = 0$ for all $n \neq 0$ and $B_n = 0$ for all odd $n \geq 3$. Therefore (5.2.12) clearly holds for $i = 0$. While when $i = k-2$, we have $G_k^{(k-2)}(x, y) = R_k^{(k-2)}(x, y) = 0$. By Lemma 5.2.5, we have $F_k^{(k-2)}(x, y) = 0$, so (5.2.12) also clearly holds for $i = k-2$. Hence we only need to prove (5.2.12) for $1 \leq i \leq k-3$. We will prove the statement by induction on k. For $k = 5$, it is easy to check that

$$\begin{aligned} F_5^{(1)}(x, x-y) + F_5^{(1)}(x, y) = R_5^{(1)}(x-y, y) &= \frac{1}{3}x^3; \\ F_5^{(2)}(x, x-y) + F_5^{(2)}(x, y) = R_5^{(2)}(x-y, y) &= -\frac{1}{3}x^3. \end{aligned}$$

Assume that

$$F^{(i)}_{k-2}(x, x-y) + F^{(i)}_{k-2}(x, y) = R^{(i)}_{k-2}(x-y, y)$$

for any i satisfying $0 \le i \le k-4$.

For any $1 \le i \le k-3$, by Lemmas 5.2.4, 5.2.5 and 5.2.6, we have

$$\begin{aligned}
& \frac{\partial^2}{\partial y^2}\left(F^{(i)}_{k}(x, x-y) + F^{(i)}_{k}(x, y)\right) \\
\overset{\text{Lemma 5.2.4}}{=} \quad & (k-2-i)(k-3-i)\left(F^{(i)}_{k-2}(x, x-y) + F^{(i)}_{k-2}(x, y)\right) \\
& -2i(k-2-i)\left(G^{(k-3-i)}_{k-2}(x, x-y) + G^{(k-3-i)}_{k-2}(x, y)\right) \\
& +i(i-1)\left(F^{(i-2)}_{k-2}(x, x-y) + F^{(i-2)}_{k-2}(x, y)\right) \\
\overset{\text{Lemma 5.2.5}}{=} \quad & (k-2-i)(k-3-i)\left(F^{(i)}_{k-2}(x, x-y) + F^{(i)}_{k-2}(x, y)\right) \\
& -2i(k-2-i)\left(F^{(k-3-i)}_{k-2}(x, x-y) + F^{(k-3-i)}_{k-2}(x, y)\right) \\
& +i(i-1)\left(F^{(i-2)}_{k-2}(x, x-y) + F^{(i-2)}_{k-2}(x, y)\right) \\
\overset{\text{Induction Hypothesis}}{=} \quad & (k-2-i)(k-3-i)R^{(i)}_{k-2}(x-y, y) \\
& -2i(k-2-i)R^{(k-3-i)}_{k-2}(x-y, y) \\
& +i(i-1)R^{(i-2)}_{k-2}(x-y, y) \\
\overset{\text{Lemma 5.2.6}}{=} \quad & \frac{\partial^2}{\partial y^2}\left(R^{(i)}_{k}(x-y, y)\right).
\end{aligned}$$

Hence,

$$F^{(i)}_{k}(x, x-y) + F^{(i)}_{k}(x, y) - R^{(i)}_{k}(x-y, y) = a_1 x^{k-3} y^1 + a_0 x^{k-2}.$$

After making the change-of-variables $x \mapsto x+y$ and $y \mapsto y$, we get

$$F^{(i)}_{k}(x+y, x) + F^{(i)}_{k}(x+y, y) - R^{(i)}_{k}(x, y) = a_1 (x+y)^{k-3} y^1 + a_0 (x+y)^{k-2}.$$

Since both $F_k^{(i)}(x+y,x)+F_k^{(i)}(x+y,y)-R_k^{(i)}(x,y)$ and $a_0(x+y)^{k-2}$ are symmetric about x and y, and $a_1(x+y)^{k-3}y^1$ is not, we have $a_1=0$, i.e.,

$$F_k^{(i)}(x,x-y)+F_k^{(i)}(x,y)-R_k^{(i)}(x-y,y)=a_0x^{k-2}.$$

Now let us consider the coefficient of x^{k-2} in the LHS. By Lemma 5.2.7, we have

$$\begin{aligned}
a_0 &= \text{coefficient of } x^{k-2} \text{ in } F_k^{(i)}(x,x-y)+F_k^{(i)}(x,y)-R_k^{(i)}(x-y,y)\\
&= \sum_{s=1}^{K-1}\left(\frac{2}{2s-1}\sum_{n=0}^{k-2s}\binom{i}{k-2s-n}\binom{n+2s-2}{n}B_n\right)+0-\frac{k-2-2i}{k-2}\\
&= A_k^{(i)}-\left(\frac{2}{2K-1}\sum_{n=0}^{k-2K}\binom{i}{k-2K-n}\binom{n+2K-2}{n}B_n\right)-\frac{k-2-2i}{k-2}\\
&\overset{\textit{Lemma } 5.2.7}{=} 0-\left(\frac{2}{k-2}\sum_{n=0}^{1}\binom{i}{1-n}\binom{n+k-3}{n}B_n\right)-\frac{k-2-2i}{k-2}\\
&= -\frac{2}{k-2}\left(iB_0+(k-2)B_1\right)-\frac{k-2-2i}{k-2}\\
&= -\frac{2}{k-2}\left(i\cdot 1+(k-2)\cdot\left(-\frac{1}{2}\right)\right)-\frac{k-2-2i}{k-2}\\
&= 0.
\end{aligned}$$

By induction, we have proven the statement for F. The result for G follows directly from Lemma 5.2.5. □

5.2.3 Proof of lemmas

In this section, we will prove all the lemmas stated in the last section.

Proof of Lemma 5.2.4. When $i=0$ or $k-2$, both sides of (5.2.6) are 0. Assume that we have $1\le i\le k-3$. Let us compare two sides of (5.2.6):

$$\text{LHS} = \frac{\partial^2}{\partial y^2}\left(F_k^{(i)}(x,y)\right)$$

$$= \sum_{s=2}^{K-1}\left(\frac{2}{2s-1}\sum_{n=0}^{k-2s}\binom{i}{k-2s-n}\binom{n+2s-2}{n}B_n\right) \times(2s-1)(2s-2)x^{2K-2s}y^{2s-3},$$

$$\text{RHS} = (k-2-i)(k-3-i)F_{k-2}^{(i)}(x,y)-2i(k-2-i)G_{k-2}^{(k-3-i)}(x,y) +i(i-1)F_{k-2}^{(i-2)}(x,y)$$

$$= (k-2-i)(k-3-i) \times\sum_{s=1}^{K-2}\left(\frac{2}{2s-1}\sum_{n=0}^{k-2-2s}\binom{i}{k-2-2s-n}\binom{n+2s-2}{n}B_n\right)x^{2K-2-2s}y^{2s-1}$$
$$-2i(k-2-i) \times\sum_{s=1}^{K-2}\left(\frac{-2}{2s-1}\sum_{n=0}^{k-2-2s}\binom{i-1}{k-2-2s-n}\binom{n+2s-2}{n}B_n\right)x^{2K-2-2s}y^{2s-1}$$
$$+i(i-1) \times\sum_{s=1}^{K-2}\left(\frac{2}{2s-1}\sum_{n=0}^{k-2-2s}\binom{i-2}{k-2-2s-n}\binom{n+2s-2}{n}B_n\right)x^{2K-2-2s}y^{2s-1}$$
$$= (k-2-i)(k-3-i) \times\sum_{s=2}^{K-1}\left(\frac{2}{2s-3}\sum_{n=0}^{k-2s}\binom{i}{k-2s-n}\binom{n+2s-4}{n}B_n\right)x^{2K-2s}y^{2s-3}$$
$$+2i(k-2-i) \times\sum_{s=2}^{K-1}\left(\frac{2}{2s-3}\sum_{n=0}^{k-2s}\binom{i-1}{k-2s-n}\binom{n+2s-4}{n}B_n\right)x^{2K-2s}y^{2s-3}$$
$$+i(i-1) \times\sum_{s=2}^{K-1}\left(\frac{2}{2s-3}\sum_{n=0}^{k-2s}\binom{i-2}{k-2s-n}\binom{n+2s-4}{n}B_n\right)x^{2K-2s}y^{2s-3}.$$

Fix any s and n, the coefficient of $B_nx^{2K-2s}y^{2s-3}$ on the RHS will be

$$\frac{2}{2s-3}\binom{i}{k-2s-n}\binom{n+2s-4}{n} \times[(k-2-i)(k-3-i)+2(i-k+2s+n)(k-2-i) +(i-k+2s+n)(i-1-k+2s+n)]$$

$$\begin{aligned}
&= \frac{2}{2s-3}\binom{i}{k-2s-n}\binom{n+2s-4}{n}(n+2s-2)(n+2s-3) \\
&= 2(2s-2)\binom{i}{k-2s-n}\binom{n+2s-4}{n}\frac{(n+2s-2)(n+2s-3)}{(2s-2)(2s-3)} \\
&= 2(2s-2)\binom{i}{k-2s-n}\binom{n+2s-2}{n},
\end{aligned}$$

which is exactly the coefficient of $B_n x^{2K-2s}y^{2s-3}$ on the LHS. Therefore, we have shown (5.2.6). The fact that

$$F_k^{(i)}(x,y) = -G_k^{(k-2-i)}(x,y)$$

directly implies (5.2.7). □

In order to prove Lemma 5.2.5, we need the following lemma, which is known as Carlitz's symmetric Bernoulli number identity [8],[33].

Lemma 5.2.8 (Carlitz)**.** *For any positive integers m, n, we have*

$$(-1)^m \sum_{k=0}^{m}\binom{m}{k}B_{n+k} = (-1)^n \sum_{k=0}^{n}\binom{n}{k}B_{m+k}. \tag{5.2.13}$$

Proof of Lemma 5.2.5. We will use induction on k to prove the result. For $k=5$, it is easy to check from the definition that

$$\begin{aligned}
F_5^{(0)}(x,y) = G_5^{(0)}(x,y) &= 0 \\
F_5^{(1)}(x,y) = G_5^{(1)}(x,y) &= \frac{1}{3}x^2y \\
F_5^{(2)}(x,y) = G_5^{(2)}(x,y) &= -\frac{1}{3}x^2y \\
F_5^{(3)}(x,y) = G_5^{(3)}(x,y) &= 0.
\end{aligned}$$

Assume that we have $F^{(i)}_{k-2}(x,y)=G^{(i)}_{k-2}(x,y)$ for all i satisfying $0\le i\le k-4$. Then by Lemma 5.2.4, we have

$$\begin{aligned}\frac{\partial^2}{\partial y^2}\Big(F^{(i)}_k(x,y)-G^{(i)}_k(x,y)\Big) &= (k-2-i)(k-3-i)\big(F^{(i)}_{k-2}(x,y)-G^{(i)}_{k-2}(x,y)\big)\\ &\quad -2i(k-2-i)\big(G^{(k-3-i)}_{k-2}(x,y)-F^{(k-3-i)}_{k-2}(x,y)\big)\\ &\quad +i(i-1)\big(F^{(i-2)}_{k-2}(x,y)-G^{(i-2)}_{k-2}(x,y)\big)\\ &= 0.\end{aligned}$$

Hence,

$$F^{(i)}_k(x,y)-G^{(i)}_k(x,y)=a_1x^{k-3}y+a_0x^{k-2}.$$

According to the definition, there are no x^{k-2}-terms in both $F^{(i)}_k(x,y)$ and $G^{(i)}_k(x,y)$, i.e., we have

$$F^{(i)}_k(x,y)-G^{(i)}_k(x,y)=a_1x^{k-3}y.$$

Now let us compare the $x^{k-3}y$-terms in $F^{(i)}_k(x,y)$ and $G^{(i)}_k(x,y)$:

$$\begin{aligned}&\text{coefficient of } x^{k-3}y \text{ in } F^{(i)}_k(x,y)\\ =\;& 2\sum_{n=0}^{k-2}\binom{i}{k-2-n}B_n\\ =\;& 2\sum_{n=0}^{k-2}\binom{i}{i-k+2+n}B_n\\ =\;& 2\sum_{j=0}^{i}\binom{i}{j}B_{j+(k-2-i)}\\ \overset{\text{Lemma 5.2.8}}{=}\;& -2\sum_{j=0}^{k-2-i}\binom{k-2-i}{j}B_{j+i}\\ =\;& -2\sum_{n=0}^{k-2}\binom{k-2-i}{n-i}B_n\end{aligned}$$

$$
\begin{aligned}
&= -2\sum_{n=0}^{k-2}\binom{k-2-i}{k-2-n}B_n \\
&= \text{coefficient of } x^{k-3}y \text{ in } G_k^{(i)}(x,y).
\end{aligned}
$$

□

Proof of Lemma 5.2.6. According to the definition of $R_k^{(i)}(x,y)$, we have

$$
\begin{aligned}
R_k^{(i)}(x-y,y) &= \frac{k-2-2i}{k-2}(x-y)^{k-2} + (-1)^{i-1}(x-y)^{k-2-i}y^i \\
&\quad +(-1)^{i-1}(x-y)^i y^{k-2-i} + \frac{k-2-2i}{k-2}y^{k-2}.
\end{aligned}
$$

By taking $\frac{\partial^2}{\partial y^2}$, we have

$$
\begin{aligned}
\frac{\partial^2}{\partial y^2}\left(R_k^{(i)}(x-y,y)\right) &= (k-2-2i)(k-3)(x-y)^{k-4} \\
&\quad +(-1)^{i-1}(k-2-i)(k-3-i)(x-y)^{k-4-i}y^i \\
&\quad -2(-1)^{i-1}(k-2-i)i(x-y)^{k-3-i}y^{i-1} \\
&\quad +(-1)^{i-1}i(i-1)(x-y)^{k-2-i}y^{i-2} \\
&\quad +(-1)^{i-1}i(i-1)(x-y)^{i-2}y^{k-2-i} \\
&\quad -2(-1)^{i-1}(k-2-i)i(x-y)^{i-1}y^{k-3-i} \\
&\quad +(-1)^{i-1}(k-2-i)(k-3-i)(x-y)^i y^{k-4-i} \\
&\quad +(k-2-2i)(k-3)y^{k-4}.
\end{aligned}
$$

In the last step, all terms except for the first and last terms are exactly the middle terms on the right-hand side of (5.2.9). Let us now compare the first and last terms. The coefficients of the first and last terms on the right-hand side of (5.2.9) are given by

$$\begin{aligned} & (k-2-i)(k-3-i)\frac{k-4-2i}{k-4} - 2i(k-2-i)\frac{k-4-2(k-3-i)}{k-4} \\ & +i(i-1)\frac{k-4-2(i-2)}{k-4} \\ = \; & k^2 - 2ki - 5k + 6i + 6 \\ = \; & (k-2-2i)(k-3), \end{aligned}$$

i.e., the first and last terms on both sides also match. Therefore, we have shown the statement. □

Proof of Lemma 5.2.7. Let $k \geq 4$ be any positive integer. We will prove the result for $A_k^{(0)}$ first. By definition, we have

$$\begin{aligned} A_k^{(0)} &= \sum_{s=1}^{\lfloor \frac{k}{2} \rfloor} \frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{0}{k-2s-n} \binom{n+2s-2}{n} B_n \\ &= \sum_{s=1}^{\lfloor \frac{k}{2} \rfloor} \frac{2}{2s-1} \binom{k-2}{k-2s} B_{k-2s}. \end{aligned}$$

When k is odd, the only nonzero term in the above expression is

$$\frac{2}{k-2}\binom{k-2}{1} B_1 = \frac{2}{k-2} \cdot (k-2) \cdot \left(-\frac{1}{2}\right) = -1,$$

i.e., when k is odd we have $A_k^{(0)} = -1$.

On the other hand, when k is even, the above expression can be written as

$$\begin{aligned} A_k^{(0)} &= \sum_{s=1}^{\lfloor \frac{k}{2} \rfloor} \frac{2}{2s-1} \binom{k-2}{k-2s} B_{k-2s} \\ &= \frac{2}{k-1} \sum_{s=1}^{\lfloor \frac{k}{2} \rfloor} \binom{k-1}{k-2s} B_{k-2s} \end{aligned}$$

$$
\begin{aligned}
&= \frac{2}{k-1}\left(\sum_{i=0}^{k-2}\binom{k-1}{i}B_i - \binom{k-1}{1}B_1\right) \\
&= \frac{2}{k-1}\left(0 - \binom{k-1}{1}B_1\right) \\
&= \frac{2}{k-1}\left(-(k-1)\cdot\left(-\frac{1}{2}\right)\right) \\
&= 1,
\end{aligned}
$$

i.e., when k is even we have $A_k^{(0)} = 1$.

Therefore, we have proven the statement for $i = 0$. Now let i be any positive integer satisfying $1 \leq i \leq k-3$. We can rewrite $A_k^{(i)}$ as follows

$$
\begin{aligned}
A_k^{(i)} &= \sum_{s=1}^{\lfloor \frac{k}{2} \rfloor} \frac{2}{2s-1} \sum_{n=0}^{k-2s} \binom{i}{k-2s-n}\binom{n+2s-2}{n} B_n \\
&= \sum_{n=0}^{k-2} \sum_{s=1}^{\lfloor \frac{k-n}{2} \rfloor} \frac{2}{2s-1}\binom{i}{k-2s-n}\binom{n+2s-2}{n} B_n.
\end{aligned}
$$

It is easy to check that $A_4^{(1)} = 0$. Now we will use induction on k, starting with $k = 4$, to prove the statement. Assume that we have $A_{k-1}^{(i)} = 0$ for all $1 \leq i \leq (k-1)-3 = k-4$. For any $0 \leq i \leq k-3$ we have

$$
\begin{aligned}
&A_k^{(i+1)} - A_k^{(i)} \\
&= \sum_{n=0}^{k-2}\left[\sum_{s=1}^{\lfloor \frac{k-n}{2} \rfloor} \frac{2}{2s-1}\left(\binom{i+1}{k-2s-n} - \binom{i}{k-2s-n}\right)\binom{n+2s-2}{n}\right] B_n \\
&= \sum_{n=0}^{k-2}\left[\sum_{s=1}^{\lfloor \frac{k-n}{2} \rfloor} \frac{2}{2s-1}\binom{i}{k-1-2s-n}\binom{n+2s-2}{n}\right] B_n,
\end{aligned}
$$

When $n = k-2$, we have

$$
\binom{i}{k-1-2s-n} = \binom{i}{1-2s} = 0 \qquad \text{for any } s \geq 1.
$$

Also when $s = \frac{k-n}{2}$ is an integer, we have

$$\binom{i}{k-1-2s-n} = \binom{i}{-1} = 0.$$

Hence,

$$\begin{aligned} A_k^{(i+1)} - A_k^{(i)} &= \sum_{n=0}^{k-2}\left[\sum_{s=1}^{\lfloor\frac{k-n}{2}\rfloor} \frac{2}{2s-1}\binom{i}{k-1-2s-n}\binom{n+2s-2}{n}\right]B_n \\ &= \sum_{n=0}^{k-3}\left[\sum_{s=1}^{\lfloor\frac{k-1-n}{2}\rfloor} \frac{2}{2s-1}\binom{i}{k-1-2s-n}\binom{n+2s-2}{n}\right]B_n \\ &= A_{k-1}^{(i)}. \end{aligned}$$

Let $i = 0$ in the above identity. We get

$$A_k^{(1)} = A_k^{(0)} + A_{k-1}^{(0)} = (-1)^k + (-1)^{k-1} = 0.$$

Similarly, the result for $A_k^{(i+1)}$ follows from the results for $A_k^{(i)}$ and $A_{k-1}^{(i)}$. □

5.3 A family of Bernoulli number identities

In this section, we will give an extension of Definition 5.2.1 and Lemma 5.2.5 for arbitrary integers i. This will allow us to derive more Bernoulli number identities.

Definition 5.3.1. Let $k = 2K + 1 \geq 5$ be an odd integer. For any integer i, we define the following two polynomials

$$\begin{aligned} F_k^{(i)}(x,y) &:= \sum_{s=1}^{K-1}\left(\frac{2}{2s-1}\sum_{n=0}^{k-2s}\binom{i}{k-2s-n}\binom{n+2s-2}{n}B_n\right)x^{2K-2s}y^{2s-1}; \\ G_k^{(i)}(x,y) &:= \sum_{s=1}^{K-1}\left(\frac{-2}{2s-1}\sum_{n=0}^{k-2s}\binom{k-2-i}{k-2s-n}\binom{n+2s-2}{n}B_n\right)x^{2K-2s}y^{2s-1}, \end{aligned} \tag{5.3.1}$$

(5.3.2)

where the binomial coefficient is defined by

$$\binom{x}{y} = \frac{\Gamma(x+1)}{\Gamma(y+1)\Gamma(x-y+1)}, \tag{5.3.3}$$

where $\Gamma(x)$ is the Gamma function.

The binomial coefficients for negative arguments are explicitly computed by the following theorem.

Theorem 5.3.2 ([23])**.** *For a negative integer n and an integer k, we have*

$$\binom{n}{k} = \begin{cases} (-1)^k \binom{-n+k-1}{k} & \text{if } k \geq 0 \\ (-1)^{n-k} \binom{-k-1}{n-k} & \text{if } k \leq n \\ 0 & \text{otherwise.} \end{cases} \tag{5.3.4}$$

These binomial coefficients satisfy the following properties.

$$\binom{x}{y} = \binom{x}{x-y} \tag{5.3.5}$$

$$\binom{x}{y}\binom{y}{z} = \binom{x}{z}\binom{x-z}{y-z} \tag{5.3.6}$$

$$\binom{x}{y} = \frac{x}{y}\binom{x-1}{y-1} \quad \text{(except } y=0\text{)} \tag{5.3.7}$$

$$\binom{x}{y} = \binom{x-1}{y} + \binom{x-1}{y-1} \quad \text{(except } x=y=0\text{)} \tag{5.3.8}$$

In the proofs of Lemmas 5.2.4 and 5.2.5, we only used the above properties of binomial coefficients along with Lemma 5.2.8 for the usual binomial coefficients. Therefore, we have

Proposition 5.3.3. *For any integer i, we have*

$$F_k^{(i)}(x,y) = G_k^{(i)}(x,y) \tag{5.3.9}$$

Comparing the coefficients on both sides, we get

Corollary 5.3.4. *For any integer s satisfying $1 \leq s \leq K$ and for any integer i, we have the following Bernoulli number identity*

$$\sum_{n=0}^{k-2s} \binom{i}{k-2s-n}\binom{n+2s-2}{n} B_n = -\sum_{n=0}^{k-2s} \binom{k-2-i}{k-2s-n}\binom{n+2s-2}{n} B_n. \tag{5.3.10}$$

5.4 Families of standard relations among double zeta values

In this section, we will prove two families of relations between motivic double zeta values of odd weight, which we call the standard relations. The first family of relations is between $\{\zeta^{\mathfrak{m}}(\mathrm{even}, \mathrm{odd})\} \cup \{\zeta^{\mathfrak{m}}(1, k-1)\}$.

Corollary 5.4.1 (One family of standard relations)**.** *For any odd integer $k \geq 5$, we have the following relation*

$$\sum_{\substack{r+s=k \\ r:\mathrm{even}}} (r-s)\zeta^{\mathfrak{m}}(r,s) + (2-k)\zeta^{\mathfrak{m}}(1,k-1) = \frac{k-7}{4}\zeta^{\mathfrak{m}}(k). \tag{5.4.1}$$

Proof of Corollary 5.4.1. On one hand, we have

$$\begin{aligned}(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2), \zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4), \ldots, \zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3))\mathcal{A}_k \\ \equiv (\zeta^{\mathfrak{m}}(2,k-2), \zeta^{\mathfrak{m}}(4,k-4), \ldots, \zeta^{\mathfrak{m}}(k-3,3)),\end{aligned}$$

where "≡" denotes congruence modulo $\mathbb{Q}\zeta^{\mathfrak{m}}(k)$. On the other hand, by Proposition 4.4.5, we have

$$\begin{aligned}\zeta^{\mathfrak{m}}(1,k-1) &\equiv -\sum_{s=1}^{\frac{k-3}{2}}\left[\binom{k-2s-1}{0}+\binom{k-2s-1}{k-2}-\delta_{k-1,2s}\right]\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)\\ &= -\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2)-\zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4)-\cdots-\zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3).\end{aligned}$$

If we denote the column vector with all entries being 1 by $\mathbf{1}$, we then have

$$\begin{aligned}&(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2),\zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4),\ldots,\zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3))(\mathcal{A}_k\mid -\mathbf{1})\\ \equiv\ &(\zeta^{\mathfrak{m}}(2,k-2),\zeta^{\mathfrak{m}}(4,k-4),\ldots,\zeta^{\mathfrak{m}}(k-3,3),\zeta^{\mathfrak{m}}(1,k-1)).\end{aligned}$$

Now we want to find a column vector in the right annihilator of the matrix $(\mathcal{A}_k \mid -\mathbf{1})$, which corresponds to a linear relation between the double zeta values

$$\{\zeta^{\mathfrak{m}}(2,k-2),\zeta^{\mathfrak{m}}(4,k-4),\ldots,\zeta^{\mathfrak{m}}(k-3,3),\zeta^{\mathfrak{m}}(1,k-1)\}.$$

Since $\mathcal{A}_k$ is invertible, we have

$$(\mathcal{A}_k\mid -\mathbf{1})v=0 \Longleftrightarrow \mathcal{A}_k^{-1}(\mathcal{A}_k\mid -\mathbf{1})v=0,$$

and the space of solutions is 1-dimensional. Now we only need to solve for

$$\mathcal{A}_k^{-1}(\mathcal{A}_k\mid -\mathbf{1})v=(I\mid -\mathcal{A}_k^{-1}\mathbf{1})v=0.$$

Each coefficient of a monomial in $F^{(i)}(x,y)$ corresponds to an entry in the inverse matrix. The rth entry in the last column, which corresponds to the rth entry of the column vector $-\mathcal{A}_k^{-1}\mathbf{1}$, is nothing but summing up all the coefficients, i.e., $-F_k^{(2r-1)}(1,1)$. By Theorem 5.2.3, we have

$$F_k^{(i)}(x+y,x)+F_k^{(i)}(x+y,y)=R_k^{(i)}(x,y).$$

Let $x = 1$, $y = 0$ and $i = 2r - 1$. We then have

$$-F_k^{(2r-1)}(1,1) = F_k^{(2r-1)}(1,0) - R_k^{(2r-1)}(1,0) = -\frac{k-2-2(2r-1)}{k-2} = \frac{4r-k}{k-2}.$$

Then $-\mathcal{A}_k^{-1}\mathbf{1}$ is a column vector with rth entry $\frac{4r-k}{k-2}$.

Since $(I \mid -\mathcal{A}_k^{-1}\mathbf{1})$ has full row rank, and one more column than row, the right annihilator of it must be 1-dimensional. Thus,

$$v = \left(\frac{k-4}{k-2}, \frac{k-8}{k-2}, \ldots, \frac{6-k}{k-2}, 1\right)^T$$

is a basis element for the right annihilator.

Therefore, we have the following relation

$$\begin{aligned} & \frac{k-4}{k-2}\zeta^{\mathfrak{m}}(2,k-2) + \frac{k-8}{k-2}\zeta^{\mathfrak{m}}(4,k-4) + \cdots + \frac{6-k}{k-2}\zeta^{\mathfrak{m}}(k-3,3) + \zeta^{\mathfrak{m}}(1,k-1) \\ \equiv\; & 0 \pmod{\zeta^{\mathfrak{m}}(k)}. \end{aligned}$$

Finally, let us compute the coefficient of $\zeta^{\mathfrak{m}}(k)$ by using Propositions 4.4.5. We have

$$\begin{aligned} & \text{LHS of (5.4.1)} \\ =\; & -\frac{1}{2}\sum_{\substack{r+s=k \\ r:\text{even}}} (r-s)\left[\binom{k-1}{r-1} + \binom{k-1}{s-1} + 1\right]\zeta^{\mathfrak{m}}(k) \\ & + \frac{2-k}{2}\left[\binom{k-1}{0} + \binom{k-1}{k-2} - 1\right]\zeta^{\mathfrak{m}}(k) \\ =\; & -\frac{1}{2}\sum_{\substack{r+s=k \\ r:\text{even}}} (r-s)\left[\binom{k-1}{r-1} + \binom{k-1}{r} + 1\right]\zeta^{\mathfrak{m}}(k) + \frac{2-k}{2}(1+k-1-1)\zeta^{\mathfrak{m}}(k) \\ =\; & -\frac{1}{2}\sum_{\substack{r+s=k \\ r:\text{even}}} (r-s)\left[\binom{k}{r} + 1\right]\zeta^{\mathfrak{m}}(k) + \frac{(2-k)(k-1)}{2}\zeta^{\mathfrak{m}}(k) \\ =\; & -\frac{1}{2}\sum_{\substack{r+s=k \\ r:\text{even}}} \left[r\binom{k}{r} - (k-r)\binom{k}{k-r}\right]\zeta^{\mathfrak{m}}(k) - \frac{1}{2}\sum_{\substack{r+s=k \\ r:\text{even}}} r\zeta^{\mathfrak{m}}(k) + \frac{1}{2}\sum_{\substack{r+s=k \\ r:\text{even}}} s\zeta^{\mathfrak{m}}(k) \end{aligned}$$

$$
\begin{aligned}
& +\frac{(2-k)(k-1)}{2}\zeta^{\mathfrak{m}}(k) \\
= \ & -\frac{k}{2}\sum_{\substack{r+s=k \\ r:\text{even}}}\left[\binom{k-1}{r-1}-\binom{k-1}{k-r-1}\right]\zeta^{\mathfrak{m}}(k)-\frac{1}{2}\left[\frac{(k-1)(k-3)}{2}\right. \\
& \left.-\frac{(k+1)(k-3)}{2}\right]\zeta^{\mathfrak{m}}(k) \\
& +\frac{(2-k)(k-1)}{2}\zeta^{\mathfrak{m}}(k) \\
= \ & -\frac{k}{2}\left[\binom{k-1}{0}-\binom{k-1}{k-2}+\binom{k-1}{k-1}\right]\zeta^{\mathfrak{m}}(k) \\
& -\frac{1}{2}\left[\frac{(k-1)(k-3)}{2}-\frac{(k+1)(k-3)}{2}\right]\zeta^{\mathfrak{m}}(k) \\
& +\frac{(2-k)(k-1)}{2}\zeta^{\mathfrak{m}}(k) \\
= \ & \frac{k-7}{4}\zeta^{\mathfrak{m}}(k).
\end{aligned}
$$

The first term in the second-to-last step comes from the binomial expansion of $(1-1)^{k-1}=0$; the 3 binomial coefficients are exactly the missing ones in the summation of the previous step. □

The second family of relations is between $\{\zeta^{\mathfrak{m}}(\text{odd},\text{even})\}\cup\{\zeta^{\mathfrak{m}}(1,k-1)\}$.

Corollary 5.4.2 (Another family of standard relations)**.** *For any odd integer $k\geq 5$, we have the following relation*

$$
(k-2)\zeta^{\mathfrak{m}}(k-2,2)+\sum_{\substack{r+s=k \\ 3\leq r\leq k-4:\text{odd}}}(r-s)\zeta^{\mathfrak{m}}(r,s)-2(k-2)\zeta^{\mathfrak{m}}(1,k-1)=\frac{3(k-3)}{4}\zeta^{\mathfrak{m}}(k). \tag{5.4.2}
$$

Proof of Corollary 5.4.2. According to Proposition 4.4.5, we have

$$
\zeta^{\mathfrak{m}}(k-2,2)
$$

$$\begin{aligned}
&\equiv (-1)^{k-2}\sum_{s=1}^{\frac{k-3}{2}}\left[\binom{k-2s-1}{k-3}+\binom{k-2s-1}{1}-\delta_{2,2s}\right]\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)\\
&= -\sum_{s=1}^{\frac{k-3}{2}}\binom{k-2s-1}{1}\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)\\
&= -\sum_{s=1}^{\frac{k-3}{2}}(k-2s-1)\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s),
\end{aligned}$$

where the first line is modulo $\zeta^{\mathfrak{m}}(k)$. Now using the decomposition results above for $\zeta^{\mathfrak{m}}(1,k-1)$ and $\zeta^{\mathfrak{m}}(k-2,2)$, we have

$$\begin{aligned}
&\text{LHS of (5.4.2)}\\
\equiv\ & 2\zeta^{\mathfrak{m}}(k-2,2)+(k-4)\zeta^{\mathfrak{m}}(k-2,2)+(k-8)\zeta^{\mathfrak{m}}(k-4,4)+\cdots\\
&+(6-k)\zeta^{\mathfrak{m}}(3,k-3)-2(k-2)\zeta^{\mathfrak{m}}(1,k-1)\\
\equiv\ & -2\sum_{s=1}^{\frac{k-3}{2}}(k-2s-1)\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)\\
&+(k-4)(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2)-\zeta^{\mathfrak{m}}(2,k-2))\\
&+(k-8)(\zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4)-\zeta^{\mathfrak{m}}(4,k-4))\\
&+\cdots+(6-k)(\zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3)-\zeta^{\mathfrak{m}}(k-3,3))\\
&+2(k-2)(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2)+\zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4)+\cdots+\zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3))\\
\equiv\ & -2\sum_{s=1}^{\frac{k-3}{2}}(k-2s-1)\zeta^{\mathfrak{m}}(2s)\zeta^{\mathfrak{m}}(k-2s)\\
&+(k-4)\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2)+(k-8)\zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4)+\cdots+(6-k)\zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3)\\
&+(k-2)(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(k-2)+\zeta^{\mathfrak{m}}(4)\zeta^{\mathfrak{m}}(k-4)+\cdots+\zeta^{\mathfrak{m}}(k-3)\zeta^{\mathfrak{m}}(3))\\
\equiv\ & 0,
\end{aligned}$$

where in the second step we use $\zeta^{\mathfrak{m}}(r,s)+\zeta^{\mathfrak{m}}(s,r)=\zeta^{\mathfrak{m}}(r)\zeta^{\mathfrak{m}}(s)-\zeta^{\mathfrak{m}}(r+s)$ and in the third step we use Corollary 5.4.1. Finally, the coefficient of $\zeta^{\mathtt{m}}(k)$ can also be computed easily by using Proposition 4.4.5, just as we did in the proof of Corollary 5.4.1. $\square$

CHAPTER 6

Double Zeta Values of Parity (odd,even)

In this chapter, we will prove two results about period polynomial relations among double zeta values of odd weight. We will also give an answer to a question asked by Zagier in [36]. At the end, we will also formulate our result in the motivic setting. The results in Sections 6.1–6.3 can also be found in [27].

6.1 Our GKZ-type result in the formal double zeta value setting

We first state our result in the formal double zeta value setting. There are two types of period polynomial relations of weight k. One comes from the odd period polynomials of weight $k-1$, and the other comes from the restricted even period polynomials of weight $k+1$.

Theorem 6.1.1 (Type I). *Let $k \geq 12$ be an even integer. To each $p \in \mathbf{W}_k^+$, we associate the coefficients $b_{r,s}$ $(r+s=k+1)$ which are defined by*

$$p(X+Y,Y) = \sum_{r+s=k+1} \binom{k-1}{r-1} b_{r,s} X^{r-1} Y^{s-2}.$$

Then

$$\sum_{\substack{r+s=k+1 \\ 4\leq r\leq k-2:\text{even}}} (b_{r,s}-b_{s,r}) Z_{r,s} \equiv 0 \qquad (\mathrm{mod}\ Z_{k+1}). \tag{6.1.1}$$

Theorem 6.1.2 (Type II)**.** *Let $k \geq 12$ be an even integer. To each $p \in \mathbf{W}_k^{-,0}$, we associate the coefficients $c_{r,s}$ $(r+s=k-1)$ which are defined by*

$$\frac{\partial}{\partial X} p(X+Y,Y) = \sum_{r+s=k-1} \binom{k-3}{r-1} c_{r,s} X^{r-1} Y^{s-1}.$$

Then

$$\sum_{\substack{r+s=k-1 \\ 4 \leq r \leq k-4:\text{even}}} (c_{r,s} - c_{s,r}) Z_{r,s} \equiv 0 \qquad (\text{mod } Z_{k-1}). \tag{6.1.2}$$

We can also show that the relations coming from Theorems 6.1.1 and 6.1.2 are actually linearly independent.

Theorem 6.1.3. *Let $k \geq 7$ be an odd integer. Up to rational multiples of $\zeta(k)$, the double zeta values*

$$\{\zeta(r,s) |\ s \text{ even},\ 4 \leq s \leq k-3,\ r+s=k\}$$

satisfy at least $\dim \mathcal{S}_{k-1}(\mathrm{SL}_2(\mathbb{Z})) + \dim \mathcal{S}_{k+1}(\mathrm{SL}_2(\mathbb{Z}))$ *linearly independent rational linear relations.*

Example 6.1.4. For $k \in \{11, 13, 15\}$, the only k for which $\dim \mathcal{S}_{k-1}(\mathrm{SL}_2(\mathbb{Z})) + \dim \mathcal{S}_{k+1}(\mathrm{SL}_2(\mathbb{Z})) = 1$, we have

$$-3\zeta(11) = 28\zeta(3,8) + 20\zeta(5,6) - 42\zeta(7,4);$$

$$-3\zeta(13) = 24\zeta(3,10) + 28\zeta(5,8) - 10\zeta(7,6) - 36\zeta(9,4);$$

$$-3\zeta(15) = 22\zeta(3,12) + 30\zeta(5,10) + 7\zeta(7,8) - 20\zeta(9,6) - 33\zeta(11,4).$$

For $k = 17$, the first case for which $\dim \mathcal{S}_{k-1}(\mathrm{SL}_2(\mathbb{Z})) = \dim \mathcal{S}_{k+1}(\mathrm{SL}_2(\mathbb{Z})) = 1$, we have

$$\begin{aligned}-23\zeta(17) &= 156\zeta(3,14) + 242\zeta(5,12)\\ &\qquad +153\zeta(7,10) - 56\zeta(9,8) - 215\zeta(11,6) - 234\zeta(13,4);\\ -597\zeta(17) &= 4004\zeta(3,14) + 6358\zeta(5,12)\\ &\qquad +4347\zeta(7,10) - 1624\zeta(9,8) - 5885\zeta(11,6) - 6006\zeta(13,4),\end{aligned}$$

where the first identity comes from $\mathcal{S}_{16}(\mathrm{SL}_2(\mathbb{Z}))$, and the second one from $\mathcal{S}_{18}(\mathrm{SL}_2(\mathbb{Z}))$.

Remark. One way to compute the coefficients of $\zeta(k)$ in the above relations is to use Proposition 3.3.1. Later, we will give another way to compute the coefficients.

6.2 Proof of Theorem 6.1.1

6.2.1 A proposition of GKZ

In [14, Proposition 2], Gangl, Kaneko and Zagier proved the following statement, which is important in understanding the connection between relations of $Z_{r,s}$ up to Z_k and the period polynomials.

Proposition 6.2.1 (Gangl-Kaneko-Zagier)**.** *Let $a_{r,s}$ and λ be rational numbers. Then the following two statements are equivalent:*

1. *The relation*

$$\sum_{r+s=k} a_{r,s} Z_{r,s} = \lambda Z_k \tag{6.2.1}$$

holds in $\mathcal{D}_k$.

2. *The generating function*

$$A(X,Y) = \sum_{r+s=k} \binom{k-2}{r-1} a_{r,s} X^{r-1} Y^{s-1} \in V_k \tag{6.2.2}$$

can be written as $H(X, X+Y) - H(X,Y)$ *for some symmetric homogeneous polynomial* $H \in \mathbb{Q}[X,Y]$ *of degree* $k-2$*, and*

$$\lambda = \frac{k-1}{2} \int_0^1 H(t, 1-t)dt. \tag{6.2.3}$$

Remark. The formula (6.2.3) gives the second explicit method of computing the coefficients of $\zeta^{\mathfrak{m}}(k)$ in the examples in the last section.

Also recall the following 5 elements in $\mathrm{PSL}_2(\mathbb{Z})$, which will be used in the proof of Theorem 6.1.1

$$\varepsilon = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \ U = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix},$$
$$T = US = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \ T' = U^2 S = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

6.2.2 Proof of Theorem 6.1.1

We now turn our attention to proving Theorems 6.1.1 and 6.1.2. We will only give a detailed proof of Theorem 6.1.1 here. Theorem 6.1.2 can be treated by the same method, so we provide the corresponding construction in a remark.

Proof of Theorem 6.1.1. Let $q = p|T$. Since p is an odd period polynomial, it must be symmetric. We have $p(X+Y, X) = p(X, X+Y)$. Let $f = q \cdot Y - q|\varepsilon \cdot X$. First we want to show that $f = f|ST'$. By a direct computation, we have

$$\begin{aligned} f|ST' - f &= (q \cdot Y - q|\varepsilon \cdot X)|ST' - (q \cdot Y - q|\varepsilon \cdot X) \\ &= q|ST' \cdot X - q|\varepsilon ST' \cdot (-(X+Y)) - (q \cdot Y - q|\varepsilon \cdot X) \\ &= (q|\varepsilon + q|ST' + q|\varepsilon ST') \cdot X + (q|\varepsilon ST' - q) \cdot Y. \end{aligned}$$

We claim that the two terms in parentheses are both zero.

$$\begin{aligned} q|\varepsilon + q|ST' + q|\varepsilon ST' &= p|T\varepsilon + p|TST' + p|T\varepsilon ST' \\ &= p(X+Y, X) + p(-Y, X) + p(-Y, -X-Y) \\ &= p(X, X+Y) - p(X, Y) + p(X+Y, Y) \\ &= 0; \\ q|\varepsilon ST' - q &= p|T\varepsilon ST' - p|T \\ &= p(-Y, -X-Y) - p(X+Y, Y) \\ &= p(X+Y, Y) - p(X+Y, Y) \\ &= 0. \end{aligned}$$

Hence we have shown that $f|ST' = f$. Now let us consider the function $f|S$. Since

$$\begin{aligned} (f|S)|\varepsilon - f|S &= (q \cdot Y - q|\varepsilon \cdot X)|S\varepsilon - (q \cdot Y - q|\varepsilon \cdot X)|S \\ &= (q|\varepsilon S\varepsilon - q|S) \cdot X + (q|S\varepsilon - q|\varepsilon S) \cdot Y \\ &= 0, \end{aligned}$$

we know that $f|S$ is a symmetric homogeneous polynomial of degree $k-1$. By applying Proposition 6.2.1 to the following identity

$$f - f|S = f|ST' - f|S,$$

the coefficients of $f - f|S$ will give us a relation between $Z_{r,s}$ $(r + s = k + 1)$ up to a scalar multiple of Z_{k+1}.

We claim that the only nonzero terms of $X^{r-1}Y^{s-1}$ appearing in $f - f|S$ are $2\binom{k-1}{r-1}(b_{r,s} - b_{s,r})X^{r-1}Y^{s-1}$ for even r satisfying $4 \leq r \leq k-2$. Since $f|S$ is symmetric, $f - f|S = f|S^2 - f|S$ contains only terms with odd powers of X between 3 and $k-3$, and those coefficients will be double the corresponding ones in f. (There are no terms of odd powers of X of degree 1 and $k-1$ since $p(1,1) = 0$ implies that q itself already does not have such terms.) According to the definition, the coefficient of $X^{r-1}Y^{s-1}$ in $f = q \cdot Y - q|\varepsilon \cdot X$ is

$$\binom{k-1}{r-1} b_{r,s} - \binom{k-1}{s-1} b_{s,r} = \binom{k-1}{r-1}(b_{r,s} - b_{s,r}).$$

Therefore, after dividing by 2, we have shown the exact relation claimed in Theorem 6.1.1. □

Remark. For the proof of Theorem 6.1.2, we need to take $q = \frac{\partial}{\partial X} p|T$ and $f = q - q|\varepsilon$. Again we have

$$f = f|ST' \Longrightarrow f - f|S = f|ST' - f|S.$$

Corollary 6.2.2. *For type I and type II, we have the following two formulas.*

- ***Type I:*** *For any $p \in \mathbf{W}_k^+$, let*

$$L_1 := \frac{p(X+Y,Y)Y - p(X+Y,X)X - p(-X+Y,Y)Y - p(Y-X,-X)X}{2}, \tag{6.2.4}$$

then

$$L_1 = \frac{f - f|S}{2}, \tag{6.2.5}$$

where $f(X,Y) = p(X+Y,X)Y - p(X+Y,Y)X$.

- ***Type II:*** *For any* $p \in \mathbf{W}_k^{-,0}$, *let* $p'(X,Y) = \frac{\partial}{\partial X} p(X,Y)$, *and*

$$L_2 := \frac{p'(X+Y,Y) - p'(X+Y,X) - p'(-X+Y,Y) + p'(Y-X,-X)}{2} \tag{6.2.6}$$

then

$$L_2 = \frac{f - f|S}{2}, \tag{6.2.7}$$

where $f(X,Y) = p'(X+Y,X) - p'(X+Y,Y)$.

Therefore, the coefficients of $Z_{r,s}$ *in the relations (6.1.1) ((6.1.2) respectively) are the coefficients of* $X^{r-1}Y^{s-1}$ *in* L_1 *(*L_2 *respectively) up to the obvious renormalization by the binomial coefficients.*

Remark. Here "the obvious renormalization by the binomial coefficients" means

$$\begin{cases} \textbf{Type I:} & \text{dividing the coefficient of } X^{r-1}Y^{s-1} \text{ in } L_1 \text{ by } \binom{k-1}{r-1}, \\ \textbf{Type II:} & \text{dividing the coefficient of } X^{r-1}Y^{s-1} \text{ in } L_2 \text{ by } \binom{k-3}{r-1}. \end{cases}$$

Proof of Corollary 6.2.2. According to the proof of Theorem 6.1.1, we know that up to the obvious renormalization by the binomial coefficients, the linear relations can be computed by $\frac{f-f|S}{2}$, where $f(X,Y) = p(X+Y,X)Y - p(X+Y,Y)X$. It can be seen from the definition that

$$L_1 = \frac{f - f|S}{2}.$$

Similarly, for type II, the linear relations can be computed by $\frac{f-f|S}{2}$, where $f(X,Y) = p'(X+Y,X) - p'(X+Y,Y)$. Again we have

$$L_2 = \frac{f - f|S}{2}.$$

□

6.2.3 Examples

Now we will provide some examples of Theorems 6.1.1 and 6.1.2. By taking the double zeta value realization, we obtain the relations among double zeta values given in Example 6.1.4. For simplicity, the period polynomials we use here are the nonhomogeneous ones, i.e., taking $y = 1$.

Example 6.2.3. The space $\mathbf{W}_{12}^{+}$ is 1-dimensional, spanned by the odd period polynomial $p(x) = 4x^9 - 25x^7 + 42x^5 - 25x^3 + 4x$. We have $p(x+1) = 4x^9 + 36x^8 + 119x^7 + 161x^6 + 21x^5 - 161x^4 - 144x^3 - 36x^2$, so the $b_{r,s}$ of the theorem are given (after multiplication by 330) by the table

r	10	9	8	7	6	5	4	3
s	3	4	5	6	7	8	9	10
$330b_{r,s}$	24	72	119	115	15	-161	-288	-216

The relations in the theorem, divided by 10, become

$$24Z_{10,3} + 28Z_{8,5} - 10Z_{6,7} - 36Z_{4,9} \equiv 0 \mod Z_{13}.$$

In the double zeta value realization, this can be written as

$$24\zeta(3,10) + 28\zeta(5,8) - 10\zeta(7,6) - 36\zeta(9,4) = -3\zeta(13). \tag{6.2.8}$$

The coefficient of $\zeta(13)$ can be obtained from (6.2.3) directly.

Example 6.2.4. The space $\mathbf{W}_{12}^{-,0}$ is 1-dimensional, spanned by the restricted even period polynomial $p(x) = x^8 - 3x^6 + 3x^4 - x^2$. We have $p'(x+1) = 8x^7 + 56x^6 + 150x^5 + 190x^4 + 112x^3 + 24x^2$, so the $c_{r,s}$ of the theorem are given (after multiplication by 63) by the table

r	8	7	6	5	4	3
s	3	4	5	6	7	8
$63c_{r,s}$	14	42	75	95	84	42

The relations in the theorem, divided by -1, become

$$28Z_{8,3} + 20Z_{6,5} - 42Z_{4,7} \equiv 0 \mod Z_{11}.$$

In the double zeta value realization, this can be written as

$$28\zeta(3,8) + 20\zeta(5,6) - 42\zeta(7,4) = -3\zeta(11). \tag{6.2.9}$$

Example 6.2.5. The space $\mathbf{W}_{16}^{-,0}$ is 1-dimensional, spanned by the restricted even period polynomial $p(x) = 2x^{12} - 7x^{10} + 11x^8 - 11x^6 + 7x^4 - 2x^2$. We have $p'(x+1) = 24x^{11} + 264x^{10} + 1250x^9 + 3330x^8 + 5488x^7 + 5824x^6 + 4050x^5 + 1850x^4 + 528x^3 + 72x^2$, so the $c_{r,s}$ of the theorem are given (after multiplication by $\frac{429}{2}$) by the table

r	12	11	10	9	8	7	6	5	4	3
s	3	4	5	6	7	8	9	10	11	12
$\frac{429}{2}c_{r,s}$	66	198	375	555	686	728	675	555	396	198

The relations in the theorem, divided by -6, become

$$22Z_{12,3} + 30Z_{10,5} + 7Z_{8,7} - 20Z_{6,9} - 33Z_{4,11} \equiv 0 \mod Z_{15}.$$

In the double zeta value realization, this can be written as

$$22\zeta(3,12) + 30\zeta(5,10) + 7\zeta(7,8) - 20\zeta(9,6) - 33\zeta(11,4) = -3\zeta(15). \tag{6.2.10}$$

Remark. The reason why we do not consider the even period polynomials $x^{10}-1$ and $x^{14}-1$ in Example 6.2.4 and Example 6.2.5, respectively, is that they give us the trivial relation.

6.2.4 The use of standard relations to answer Zagier's question

Let us see how our relations (6.1.1) and (6.1.2) are related to Zagier's matrix $\mathcal{B}_k$, which is defined by using Proposition 3.3.1. Let us first demonstrate the method through an example. When $k=11$, $\mathcal{B}_k$ is the following matrix defined by Euler's decomposition formula:

$$\begin{pmatrix} \zeta(9,2) \\ \zeta(7,4) \\ \zeta(5,6) \\ \zeta(3,8) \\ \zeta(1,10) \end{pmatrix} = \begin{pmatrix} -2 & -4 & -6 & -8 & 27 \\ 0 & -4 & -20 & -84 & \frac{329}{2} \\ 0 & 0 & -21 & -126 & \frac{461}{2} \\ 0 & -6 & -15 & -36 & 82 \\ -1 & -1 & -1 & -1 & 5 \end{pmatrix} \begin{pmatrix} \zeta(8)\zeta(3) \\ \zeta(6)\zeta(5) \\ \zeta(4)\zeta(7) \\ \zeta(2)\zeta(9) \\ \zeta(11) \end{pmatrix} = \mathcal{B}_{11} \begin{pmatrix} \zeta(8)\zeta(3) \\ \zeta(6)\zeta(5) \\ \zeta(4)\zeta(7) \\ \zeta(2)\zeta(9) \\ \zeta(11) \end{pmatrix}.$$

Let us consider the following submatrix $\mathcal{B}_{11}^{(1)}$ of $\mathcal{B}_{11}$. This is a little different from our matrix $\mathcal{A}'_{11}$.

$$\begin{pmatrix} \begin{array}{:cccc:} \hdashline -2 & -4 & -6 & -8 \\ 0 & -4 & -20 & -84 \\ 0 & 0 & -21 & -126 \\ 0 & -6 & -15 & -36 \\ \hdashline \end{array} & \begin{array}{c} 27 \\ \frac{329}{2} \\ \frac{461}{2} \\ 82 \end{array} \\ \begin{array}{cccc} -1 & -1 & -1 & -1 \end{array} & 5 \end{pmatrix}$$

Since this submatrix $\mathcal{B}_5^{(1)}$ corresponds to the linear expressions of $\{\zeta(9,2),\zeta(7,4),\zeta(5,6),\zeta(3,8)\}$ in terms of $\{\zeta(8)\zeta(3),\zeta(6)\zeta(5),\zeta(4)\zeta(7),\zeta(2)\zeta(9)\}$

up to scalar multiples of $\zeta(11)$, the relation (6.2.9) can be translated into the fact that the vector $(0, -42, 20, 28)$ lies in the kernel of $\mathcal{B}_5^{(1)}$. In general, the above argument proves the following statement.

Proposition 6.2.6. *Let $k \geq 5$ be an odd integer. Let $\mathcal{B}_k^{(1)}$ be the $(\frac{k-3}{2} \times \frac{k-3}{2})$-minor of $\mathcal{B}_k$ obtained by deleting the last columns and the last row of $\mathcal{B}_k$. Then the vectors obtained from the coefficients of $Z_{r,s}$ in the linear relations (6.1.1) and (6.1.2) belong to the kernel of $\mathcal{B}_k^{(1)}$.*

Now let us see how to use our relation (6.2.9) to get Zagier's relation

$$-6\zeta(1,10) + 17\zeta(3,8) + 13\zeta(5,6) - 27\zeta(7,4) + 3\zeta(9,2) = 0. \tag{6.2.11}$$

Or more generally for any odd weight $k \geq 11$, let us see how to use our relations from Theorems 6.1.1 and 6.1.2 to get nontrivial elements in the kernel of $\mathcal{B}_k$.

Recall from Corollary 5.4.2 that for any odd integer $k \geq 5$, we have the following standard relation

$$(k-2)\zeta^{\mathfrak{m}}(k-2,2) + \sum_{\substack{r+s=k \\ 3 \leq r \leq k-4:\text{ odd}}} (r-s)\zeta^{\mathfrak{m}}(r,s) - 2(k-2)\zeta^{\mathfrak{m}}(1,k-1) = \frac{3(k-3)}{4}\zeta^{\mathfrak{m}}(k). \tag{6.2.12}$$

Example 6.2.7. The first few standard relations of MZVs in lower weights are listed below.

$$\begin{aligned}
\frac{3}{2}\zeta(5) &= -6\zeta(1,4) + 3\zeta(3,2); \\
3\zeta(7) &= -10\zeta(1,6) - \zeta(3,4) + 5\zeta(5,2); \\
\frac{9}{2}\zeta(9) &= -14\zeta(1,8) - 3\zeta(3,6) + \zeta(5,4) + 7\zeta(7,2);
\end{aligned}$$

$$\begin{aligned}
6\zeta(11) &= -18\zeta(1,10) - 5\zeta(3,8) - \zeta(5,6) + 3\zeta(7,4) + 9\zeta(9,2); \\
\frac{15}{2}\zeta(13) &= -22\zeta(1,12) - 7\zeta(3,10) - 3\zeta(5,8) + \zeta(7,6) + 5\zeta(9,4) + 11\zeta(11,2); \\
9\zeta(15) &= -26\zeta(1,14) - 9\zeta(3,12) - 5\zeta(5,10) - \zeta(7,8) \\
&\qquad +3\zeta(9,6) + 7\zeta(11,4) + 13\zeta(13,2).
\end{aligned}$$

In particular, in weight 11, we have both the standard relation in weight 11 and our relation (6.2.9)

$$6\zeta(11) = -18\zeta(1,10) - 5\zeta(3,8) - \zeta(5,6) + 3\zeta(7,4) + 9\zeta(9,2);$$
$$-3\zeta(11) = 28\zeta(3,8) + 20\zeta(5,6) - 42\zeta(7,4).$$

Now we can easily see that by canceling $\zeta(11)$ from the above two relations, we get exactly Zagier's relation (6.2.11)

$$-6\zeta(1,10) + 17\zeta(3,8) + 13\zeta(5,6) - 27\zeta(7,4) + 3\zeta(9,2) = 0.$$

In general, for any odd integer $k \geq 11$, by cancelling $\zeta(k)$ from both the standard relation of weight k and a weight k relation obtained from Theorem 6.1.1 or Theorem 6.1.2, we will get a nontrivial element in the left kernel of $\mathcal{B}_k$.

6.3 Proof of Theorem 6.1.3

6.3.1 Proof of Theorem 6.1.3

In this section, we will prove that the linear relations obtained from Theorems 6.1.1 and 6.1.2 are all linearly independent.

The proof is based on the following injective map (cf. [36, (41)]) considered by Zagier.

$$\mathbf{W}_{k-1}^{+} \oplus \mathbf{W}_{k+1}^{-,0} \to \ker(\mathcal{B}_k^T), \tag{6.3.1}$$

where $f(x, y) \in \mathbf{W}_{k-1}^{+}$ maps to the associated vector of $f(x, y)$ and $g(x, y) \in \mathbf{W}_{k+1}^{-,0}$ maps to the associated vector of $\frac{\partial}{\partial x} g(x, y)$. According to the definition of the above map, any element in the image of $\mathbf{W}_{k-1}^{+} \oplus \mathbf{W}_{k+1}^{-,0}$ always has zero as its last entry. Hence this map naturally defines an injective map by deleting the last entry

$$\mathbf{W}_{k-1}^{+} \oplus \mathbf{W}_{k+1}^{-,0} \to \ker((\mathcal{B}_k^{(1)})^T). \tag{6.3.2}$$

We need the following lemma to relate our linear relations with the image of the above map.

Lemma 6.3.1. *The polynomials L_1 and L_2 in Corollary 6.2.2 can also be computed as follows.*

$$L_1 = L_1' := \frac{p(Y, X+Y)(X+Y) - p(Y, -X+Y)(-X+Y)}{2} \tag{6.3.3}$$

$$L_2 = L_2' := \frac{p'(Y, X+Y) - p'(Y, -X+Y)}{2} \tag{6.3.4}$$

Proof of Lemma 6.3.1.

Type I: For any $p \in W_k^+$, we have $p(X, Y) = p(Y, X)$. Therefore, we have $p(X+Y, Y)Y = p(Y, X+Y)Y$ and $p(-X+Y, Y)Y = p(Y, -X+Y)Y$. Then

$$\begin{aligned} & 2(L_1' - L_1) \\ = \; & X\big(\big(p(Y, X+Y) + p(X+Y, X)\big) + \big(p(Y, -X+Y) + p(Y-X, -X)\big)\big) \end{aligned}$$

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

- **Type II:** For any $p \in W_k^{-,0}$, we have

$$p(X, X+Y) + p(X+Y, Y) + p(Y, X) = 0.$$

Taking partial derivatives with respect to Y term by term, we have

$$\frac{\partial}{\partial Y} p(X, X+Y) = -\frac{\partial}{\partial Y} p(Y+X, X) = -p'(Y+X, X), \tag{6.3.5}$$

$$\frac{\partial}{\partial Y} p(X+Y, Y) = p'(X+Y, Y) - p'(Y, X+Y), \tag{6.3.6}$$

$$\frac{\partial}{\partial Y} p(Y, X) = p'(Y, X). \tag{6.3.7}$$

Summing over all the three terms above, we get

$$p'(Y, X+Y) - p'(X+Y, Y) + p'(X+Y, X) = p'(Y, X). \tag{6.3.8}$$

Therefore,

$$
\begin{aligned}
& 2(L_2' - L_2) \\
=\ & \Big(p'(Y, X+Y) - p'(X+Y, Y) + p'(X+Y, X)\Big) \\
& -\Big(p'(Y, -X+Y) - p'(-X+Y, Y) + p'(-X+Y, -X)\Big) \\
=\ & p'(Y, X) - p'(Y, -X) \\
=\ & 0.
\end{aligned}
$$

Hence we have proven the lemma. □

Now we are ready to prove the linear independence of the rational linear relations obtained from Theorems 6.1.1 and 6.1.2.

Proof of Theorem 6.1.3. First, we relate those the linear relations obtained from Theorem 6.1.1 and 6.1.2 to the images (6.3.2) computed by Zagier.

- **Type I:** For any $p \in \mathbf{W}_k^+$, let us assume that $p(X,Y) = \sum_{r \text{ odd}} \alpha_{r,s} X^r Y^s$. Notice that in this case, we have $r+s = k-2$. Then

$$\begin{aligned} L_1' &= \frac{p(Y,X+Y)(X+Y) - p(Y,-X+Y)(-X+Y)}{2} \\ &= \frac{1}{2}\Bigg(\sum_{r \text{ odd}} \alpha_{r,s} Y^r (X+Y)^{s+1} - \sum_{r \text{ odd}} \alpha_{r,s} Y^r (-X+Y)^{s+1} \Bigg) \\ &= \sum_{r \text{ odd}} \sum_{i \text{ odd}} \alpha_{r,s} \binom{s+1}{i} X^i Y^{k-1-i}. \end{aligned}$$

  Let us define two $(\frac{k-2}{2} \times \frac{k-2}{2})$-matrices $D_1^{(k)}$ and $B_1^{(k)}$ by

$$(D_1^{(k)})^{-1} = \operatorname{diag}\left(\binom{k-1}{2i-1} \right)_{1 \le i \le \frac{k-2}{2}}, \qquad (B_1^{(k)})_{ij} = \binom{2j}{2i-1}. \tag{6.3.9}$$

  By the above computation, we can see that left multiplication by $B_1^{(k)}$ of $(\alpha_{r,s})^T$ gives us a renormalization of $(\alpha_{r,s})^T$ by a factor of $\binom{s+1}{i}$ and further left multiplication by $D_1^{(k)}$ gives us the obvious renormalization by binomial coefficients. Therefore, by Corollary 6.2.2 and Lemma 6.3.1, the column vectors $D_1^{(k)} B_1^{(k)} (\alpha_{r,s})^T$ give us the coefficients of the rational linear relations from Theorem 6.1.1.

- **Type II:** For any $p \in \mathbf{W}_k^{-,0}$, let us assume that $p'(X,Y) = \sum_{r \text{ odd}} \beta_{r,s} X^r Y^s$. Note that in this case, we have $r+s = k-3$. Then

$$L_2' = \frac{p'(Y,X+Y) - p'(Y,-X+Y)}{2}$$

$$= \frac{1}{2}\left(\sum_{r \text{ odd}} \beta_{r,s} Y^r (X+Y)^s - \sum_{r \text{ odd}} \beta_{r,s} Y^r (-X+Y)^s \right)$$
$$= \sum_{r \text{ odd}} \sum_{i \text{ odd}} \beta_{r,s} \binom{s}{i} X^i Y^{k-3-i}$$

Let us define two $(\frac{k-4}{2} \times \frac{k-4}{2})$-matrices $D_2^{(k)}$ and $B_2^{(k)}$ by

$$(D_2^{(k)})^{-1} = \operatorname{diag}\left(\binom{k-3}{2i-1} \right)_{1 \le i \le \frac{k-4}{2}}, \qquad (B_2^{(k)})_{ij} = \binom{2j}{2i-1}. \quad (6.3.10)$$

Similarly, we can see that left multiplication by $B_2^{(k)}$ of $(\beta_{r,s})^T$ gives us a renormalization by a factor of $\binom{s}{i}$ and further left multiplication by $D_2^{(k)}$ gives us the obvious renormalization by binomial coefficients. Therefore, by Corollary 6.2.2 and Lemma 6.3.1, the column vectors $D_2^{(k)} B_2^{(k)} (\beta_{r,s})^T$ gives us the coefficients of the rational linear relations from Theorem 6.1.2.

For a fixed odd weight k, according to the definition of $D_1^{(k)}, D_2^{(k)}, B_1^{(k)}, B_2^{(k)}$, we have

$$D_1^{(k-1)} = D_2^{(k+1)}, \qquad B_1^{(k-1)} = B_2^{(k+1)}. \quad (6.3.11)$$

Moreover, $D_1^{(k)}, D_2^{(k)}$ are always invertible diagonal matrices, and $B_1^{(k)}, B_2^{(k)}$ are always invertible upper triangular matrices. The injectivity of (6.3.2) (i.e., the linear independence of $(\alpha_{r,s})^T$'s and $(\beta_{r,s})^T$'s) implies that for a fixed odd weight k, all the rational linear relations of Theorems 6.1.1 and 6.1.2 are linearly independent. Therefore, we have proven Theorem 6.1.3. □

Remark. The matrices $D_1^{(k)}, D_2^{(k)}, B_1^{(k)}, B_2^{(k)}$ are similar to the ones defined in [1, Proposition 3.3].

6.3.2 Examples

Example 6.3.2. Here we list two examples in weights 11 and 13.

- $N = 11$:

  In this case, we only have the following linear relation of type II coming from $\mathbf{W}_{12}^{-,0}$:

$$3\zeta(11) = 0\zeta(9,2) + 42\zeta(7,4) - 20\zeta(5,6) - 28\zeta(3,8).$$

  In this case,

$$D_2^{(12)} = \begin{pmatrix} \frac{1}{9} & 0 & 0 & 0 \\ 0 & \frac{1}{84} & 0 & 0 \\ 0 & 0 & \frac{1}{126} & 0 \\ 0 & 0 & 0 & \frac{1}{36} \end{pmatrix}, \quad B_2^{(12)} = \begin{pmatrix} 2 & 4 & 6 & 8 \\ 0 & 4 & 20 & 56 \\ 0 & 0 & 6 & 56 \\ 0 & 0 & 0 & 8 \end{pmatrix},$$

  and we have

$$D_2^{(12)} B_2^{(12)} (4, -9, 6, -1)^T = \left(0, \frac{1}{3}, -\frac{10}{63}, -\frac{2}{9}\right)^T = \frac{1}{126}(0, 42, -20, -28)^T.$$

- $N = 13$:

  In this case, we only have the following linear relation of type I coming from $\mathbf{W}_{12}^{+}$:

$$-3\zeta(13) = 0\zeta(11,2) - 36\zeta(9,4) - 10\zeta(7,6) + 28\zeta(5,8) + 24\zeta(3,10).$$

In this case,

$$D_1^{(12)} = \begin{pmatrix} \frac{1}{11} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{165} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{462} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{330} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{55} \end{pmatrix}, \quad B_1^{(12)} = \begin{pmatrix} 2 & 4 & 6 & 8 & 10 \\ 0 & 4 & 20 & 56 & 120 \\ 0 & 0 & 6 & 56 & 252 \\ 0 & 0 & 0 & 8 & 120 \\ 0 & 0 & 0 & 0 & 10 \end{pmatrix},$$

and we have

$$\begin{aligned} & D_1^{(12)} B_1^{(12)} (4, -25, 42, -25, 4)^T \\ = & \left(0, -\frac{12}{11}, -\frac{10}{33}, \frac{28}{33}, \frac{8}{11}\right)^T \\ = & \frac{1}{33}(0, -36, -10, 28, 24)^T. \end{aligned}$$

6.4 Our GKZ-type result in the motivic setting

Since Euler's decomposition formula also holds in the motivic setting, and Theorems 6.1.1 and 6.1.2 are obtained by studying kernel of the matrix coming from this decomposition formula, we have the following motivic versions of the theorems, and their proofs are exactly the same.

Theorem 6.4.1 (Type I)**.** *Let $k \geq 12$ be an even integer. To each $p \in \mathbf{W}_k^+$, we associate the coefficients $b_{r,s}$ $(r + s = k + 1)$ which are defined by*

$$p(X + Y, Y) = \sum_{r+s=k+1} \binom{k-1}{r-1} b_{r,s} X^{r-1} Y^{s-2}.$$

Then

$$\sum_{\substack{r+s=k+1 \\ 4 \leq r \leq k-2 \text{ even}}} (b_{r,s} - b_{s,r}) \zeta^{\mathfrak{m}}(s, r) \equiv 0 \pmod{\zeta^{\mathfrak{m}}(k+1)}. \tag{6.4.1}$$

Theorem 6.4.2 (Type II)**.** *Let $k \geq 12$ be an even integer. To each $p \in \mathbf{W}_k^{-,0}$, we associate the coefficients $c_{r,s}$ $(r+s=k-1)$ which are defined by*

$$\frac{\partial}{\partial X}p(X+Y,Y) = \sum_{r+s=k-1} \binom{k-3}{r-1} c_{r,s} X^{r-1} Y^{s-1}.$$

Then

$$\sum_{\substack{r+s=k-1 \\ 4 \leq r \leq k-4 \ even}} (c_{r,s} - c_{s,r}) \zeta^{\mathfrak{m}}(s,r) \equiv 0 \qquad (\bmod\ \zeta^{\mathfrak{m}}(k-1)). \tag{6.4.2}$$

Theorem 6.4.3. *Let $k \geq 7$ be an odd integer. Up to rational multiples of $\zeta^{\mathfrak{m}}(k)$, the motivic double zeta values $\{\zeta^{\mathfrak{m}}(r,s) |\ s$ even, $4 \leq s \leq k-3,\ r+s=k\}$ satisfy at least $\dim \mathcal{S}_{k-1}(\mathrm{SL}_2(\mathbb{Z})) + \dim \mathcal{S}_{k+1}(\mathrm{SL}_2(\mathbb{Z}))$ linearly independent rational linear relations.*

CHAPTER 7

Motivic MZVs of Higher Depth

Throughout this chapter, we assume that the weight k and depth r satisfy the condition $k \equiv r \pmod 2$.

7.1 Tasaka's result in the totally odd case

7.1.1 Operator ∂_p and matrix $\mathcal{C}_{N,r}$

Recall from Definition 4.3.1 that for each odd integer $p > 1$, we have a derivation

$$D_p : \mathcal{H} \to \mathcal{L}_p \otimes \mathcal{H}$$

If we consider the depth filtration on $\mathcal{H}$, we have

$$D_p : \mathfrak{D}_r \mathcal{H} \to \mathfrak{D}_1 \mathcal{L}_p \otimes \mathfrak{D}_{r-1} \mathcal{H} + \mathcal{L}_p \otimes \mathfrak{D}_{r-2} \mathcal{H},$$

where as in the proof of Proposition 4.3.2, the evaluation of D_p on a motivic iterated integral can be broken into a sum of tensor products of motivic iterated integrals of lower depth, those landing in the first term corresponding to subsequences of depth 1. Therefore, D_p induces a map

$$\mathrm{gr}_r^{\mathfrak{D}} D_p : \mathrm{gr}_r^{\mathfrak{D}} \mathcal{H}_k \to \mathfrak{D}_1 \mathcal{L}_p \otimes \mathrm{gr}_{r-1}^{\mathfrak{D}} \mathcal{H}_{k-p}.$$

As before, let us denote by ξ_p the image of $\zeta^{\mathfrak{m}}(p)$ in the space $\mathcal{L}_p$. Then the derivation operator ∂_p is defined to be

$$\partial_p := (\xi_p^\vee \otimes 1) \circ \mathrm{gr}_r^{\mathfrak{D}} D_p : \mathrm{gr}_r^{\mathfrak{D}} \mathcal{H}_k \to \mathrm{gr}_{r-1}^{\mathfrak{D}} \mathcal{H}_{k-p},$$

where $\xi_p^\vee$ maps the basis element ξ_p of the 1-dimensional vector space $\mathfrak{D}_1\mathcal{L}_p$ to 1. By proving that

$$D_p(\mathfrak{D}_r\mathcal{H}^{\mathrm{odd}}) \subset \mathfrak{D}_1\mathcal{L}_p \otimes \mathfrak{D}_{r-1}\mathcal{H}^{\mathrm{odd}} + \mathcal{L}_p \otimes \mathfrak{D}_{r-2}\mathcal{H},$$

Brown (cf. [4, Proposition 10.1]) showed that this ∂_p is also well defined upon restriction to $\mathcal{H}^{\mathrm{odd}}$, i.e., we have

$$\partial_p : \mathrm{gr}_r^{\mathfrak{D}} \mathcal{H}_k^{\mathrm{odd}} \to \mathrm{gr}_{r-1}^{\mathfrak{D}} \mathcal{H}_{k-p}^{\mathrm{odd}}.$$

Here we use the same symbol ∂_p for both cases, and do not distinguish them.

Definition 7.1.1 ($S_{k,r}$ and $\mathrm{Total}_{k,r}$)**.** Define

$$S_{k,r} = \{(n_1, n_2, \dots, n_r) : n_i \geq 3 \text{ an odd integer for all } i, n_1 + n_2 + \cdots + n_r = k\}$$

to be the totally odd indexing set, and define

$$\mathrm{Total}_{k,r} = \{(n_1, n_2, \dots, n_r) : n_i \geq 1 \text{ an integer for all } i, n_1 + n_2 + \cdots + n_r = k\}$$

to be the total indexing set.

Definition 7.1.2 ($c\binom{m_1,\dots,m_r}{n_1,\dots,n_r}$)**.** For any $(m_1, \dots, m_r) \in S_{k,r}$ and any $(n_1, \dots, n_r) \in \mathrm{Total}_{k,r}$, let us define

$$c\binom{m_1,\dots,m_r}{n_1,\dots,n_r} = \partial_{m_r} \circ \partial_{m_{r-1}} \circ \cdots \circ \partial_{m_1}(\zeta_{\mathfrak{D}}^{\mathfrak{m}}(n_1, \dots, n_r)) \in \mathbb{Q}. \tag{7.1.1}$$

Definition 7.1.3 ($\mathcal{C}_{k,r}$)**.** For integers $k > r > 0$, we define the $|S_{k,r}| \times |S_{k,r}|$ matrix $\mathcal{C}_{k,r}$ by

$$\mathcal{C}_{k,r} = \left(c\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r} \right)_{\substack{(m_1,\ldots,m_r)\in S_{k,r} \\ (n_1,\ldots,n_r)\in S_{k,r}}} \tag{7.1.2}$$

Note that we do not specify the ordering of the indexing set $S_{k,r}$ here. This matrix $\mathcal{C}_{k,r}$ led Brown to make the following three conjectures (cf. [4]).

Conjecture 7.1.4 (Brown)**.** *A $\mathbb{Q}$-linear combination ξ of totally odd depth-graded motivic MZVs of weight k and depth r is zero if and only if it satisfies $\partial_{m_r} \circ \partial_{m_{r-1}} \circ \cdots \circ \partial_{m_1}(\xi) = 0$ for all $(m_1, \ldots, m_r) \in S_{k,r}$, i.e., its corresponding column vector lies in* $\ker(\mathcal{C}^T_{k,r})$.

Remark. Conjecture 7.1.4 is true for $r = 2, 3$ from Zagier [39], and Goncharov [17].

Conjecture 7.1.5 (Brown)**.** *The rank of the matrix $\mathcal{C}_{k,r}$ is equal to the dimension of the $\mathbb{Q}$-vector space spanned by all totally odd (motivic) MZVs of weight k and depth r.*

Conjecture 7.1.6 (Brown)**.** *The generating series of* rank $\mathcal{C}_{k,r}$ *is given by*

$$1 + \sum_{k>r>0} \text{rank } \mathcal{C}_{k,r} x^k y^r = \frac{1}{1 - \mathbb{O}(x)y + \mathbb{S}(x)y^2}.$$

Combining Conjectures 7.1.5 and 7.1.6 leads to Conjecture 4.2.2, the motivic totally odd Broadhurst-Kreimer conjecture.

7.1.2 Polynomial representation of the Ihara action

We now recall the polynomial representation of the Ihara action studied by Brown in [4, Section 6.1].

Definition 7.1.7 (linearized Ihara action)**.** Define

$$\underline{\circ}\ : \mathbb{Q}[x_1,\dots,x_r]\otimes_{\mathbb{Q}}\mathbb{Q}[x_1,\dots,x_s]\to\mathbb{Q}[x_1,\dots,x_{r+s}]$$

to be given by

$$\begin{aligned} & (f\ \underline{\circ}\ g)(x_1,\dots,x_{r+s}) \\ = & \sum_{i=0}^{s} f(x_{i+1}-x_i,\dots,x_{i+r}-x_i)g(x_1,\dots,\widehat{x}_{i+1},\dots,x_{r+s}) \\ & +(-1)^{\deg(f)+r}\sum_{i=1}^{s} f(x_{i+r-1}-x_{i+r},\dots,x_i-x_{i+r})g(x_1,\dots,\widehat{x}_i,\dots,x_{r+s}) \end{aligned}$$

for any homogeneous polynomials f and g, where $x_0=0$ by convention. We call this operation the linearized Ihara action.

Remark. This is the polynomial representation of the depth-graded version of the linearization of the Ihara action (4.1.3) (see the remark after Definition 7.4.5 for details).

This linearized Ihara action defined above is dual to the formula (4.3.1) in the following sense (cf. [4, Proof of Proposition 3.2]). For any odd $p\geq 3$ and integers $m_1,\dots,m_r$, the corresponding coefficients in

$$\begin{aligned} \partial_p\zeta^{\mathfrak{m}}_{\mathfrak{D}}(m_1,\dots,m_r) &= \sum a_{n_1,\dots,n_{r-1}}\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1,\dots,n_{r-1}) \\ x_1^{m_1-1}\ \underline{\circ}\ (x_1^{m_2-1}\cdots x_{r-1}^{m_r-1}) &= \sum b_{n_1,\dots,n_{r-1}}x_1^{p-1}x_2^{n_1-1}\cdots x_r^{n_{r-1}-1} \end{aligned}$$

are the same, i.e., $a_{n_1,\dots,n_{r-1}}=b_{n_1,\dots,n_{r-1}}$ for all $n_i\geq 1$ satisfying $n_1+\cdots+n_{r-1}+p=m_1+\cdots+m_r$. Therefore, for any $(m_1,\dots,m_r)\in S_{k,r}$ and any $(n_1,\dots,n_r)\in\mathrm{Total}_{k,r}$, the number

$$c\binom{m_1,\dots,m_r}{n_1,\dots,n_r}$$

defined in (7.1.1) by using r consecutive ∂'s coincides with the coefficient of $x_1^{n_1-1}\cdots x_r^{n_r-1}$ in

$$x_1^{m_1-1}\,\underline{\circ}\,(\cdots x_1^{m_{r-2}-1}\,\underline{\circ}\,(x_1^{m_{r-1}-1}\,\underline{\circ}\,x_1^{m_r-1})\cdots).$$

In other words, the matrices $\mathcal{C}_{k,r}$ can also be computed by using the linearized Ihara action.

7.1.3 Product formula by Tasaka

The following elements are the generalizations of the elements $e\binom{m_1,m_2}{n_1,n_2}$ defined in (4.3.2). These elements give us a decomposition of $\mathcal{C}_{k,r}$ into a product of $r-1$ (square) matrices.

Recall that the integer $b^m_{n,n'}$ $(n,n',m\in\mathbb{Z})$ defined in Section 4.3 is given by

$$b^m_{n,n'}=(-1)^n\binom{m-1}{n-1}+(-1)^{n'-m}\binom{m-1}{n'-1},$$

where $\binom{n}{m}=0$ for each $m<0$.

Definition 7.1.8. For $r>1$ and r-tuples of positive integers $(m_1,\ldots,m_r)$ and $(n_1,\ldots,n_r)$, we define

$$e\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r}=\delta\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r}+\sum_{i=1}^{r-1}\delta\binom{m_2,\ldots,m_i,m_{i+2},\ldots,m_r}{n_1,\ldots,n_{i-1},n_{i+2},\ldots,n_r}b^{m_1}_{n_i,n_{i+1}}\in\mathbb{Z},\tag{7.1.3}$$

and we let $e\binom{m_1}{n_1}=\delta\binom{m_1}{n_1}$.

By [35, (3.3) and Lemma 3.1], the number $e\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r}$ can be computed directly from the linearized Ihara action (cf. Definition 7.1.7) as follows:

$$x_1^{m_1-1}\,\underline{\circ}\,(x_1^{m_2-1}\cdots x_{r-1}^{m_r-1})$$

$$
\begin{aligned}
&= x_1^{m_1-1}\cdots x_r^{m_r-1} \\
&\quad + \sum_{i=1}^{r-1}(x_{i+1}-x_i)^{m_1-1}(x_1^{m_2-1}\cdots x_i^{m_{i+1}-1}x_{i+2}^{m_{i+2}-1}\cdots x_r^{m_r-1} \\
&\qquad\qquad -x_1^{m_2-1}\cdots x_{i-1}^{m_i-1}x_{i+1}^{m_{i+1}-1}\cdots x_r^{m_r-1}) \\
&= x_1^{m_1-1}\cdots x_r^{m_r-1} + \sum_{i=1}^{r-1} x_1^{m_2-1}\cdots x_{i-1}^{m_i-1}x_{i+2}^{m_{i+2}-1}\cdots x_r^{m_r-1} \\
&\quad \times \sum_{\substack{n_i+n_{i+1}=m_1+m_{i+1}\\ n_i,n_{i+1}\geq 1}} \left((-1)^{m_1-n_{i+1}}\binom{m_1-1}{n_{i+1}-1} - (-1)^{n_i-1}\binom{m_1-1}{n_i-1}\right)x_i^{n_i-1}x_{i+1}^{n_{i+1}-1} \\
&= \sum_{\substack{n_1+\cdots+n_r=m_1+\cdots+m_r\\ n_1,\ldots,n_r\geq 1}} e\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r}x_1^{n_1-1}\cdots x_r^{n_r-1}. \qquad (7.1.4)
\end{aligned}
$$

Recursively applying (7.1.4) gives us the product formula:

$$
\begin{aligned}
\mathcal{C}_{k,r} &= \left(\delta\binom{m_1,\ldots,m_{r-2}}{n_1,\ldots,n_{r-2}}e\binom{m_{r-1},m_r}{n_{r-1},n_r}\right)_{\substack{(m_1,\ldots,m_r)\in S_{k,r}\\ (n_1,\ldots,n_r)\in \mathrm{Total}_{k,r}}} \\
&\quad \cdot\prod_{i=3}^{r-1}\left(\delta\binom{m_1,\ldots,m_{r-i}}{n_1,\ldots,n_{r-i}}e\binom{m_{r-i+1},\ldots,m_r}{n_{r-i+1},\ldots,n_r}\right)_{\substack{(m_1,\ldots,m_r)\in \mathrm{Total}_{k,r}\\ (n_1,\ldots,n_r)\in \mathrm{Total}_{k,r}}} \\
&\quad \cdot\left(e\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r}\right)_{\substack{(m_1,\ldots,m_r)\in \mathrm{Total}_{k,r}\\ (n_1,\ldots,n_r)\in S_{k,r}}}, \qquad (7.1.5)
\end{aligned}
$$

where the first matrix computes $x_1^{m_1-1} \,\underline{\circ}\, (\cdots x_1^{m_{r-2}-1} \,\underline{\circ}\, (x_1^{m_{r-1}-1} \,\underline{\circ}\, x_1^{m_r-1})\cdots)$ as a linear combination of monomials in $x_1^{m_1-1} \,\underline{\circ}\, (\cdots x_1^{m_{r-2}-1} \,\underline{\circ}\, (x_1^{n_1}x_2^{n_2})\cdots)$, the second matrix computes $x_1^{m_1-1} \,\underline{\circ}\, (\cdots x_1^{m_{r-2}-1} \,\underline{\circ}\, (x_1^{n_1}x_2^{n_2})\cdots)$ as a linear combination of monomials in $x_1^{m_1-1} \,\underline{\circ}\, (\cdots x_1^{m_{r-3}-1} \,\underline{\circ}\, (x_1^{n_1}x_2^{n_2}x_3^{n_3})\cdots)$, $\cdots$, and the last matrix computes $x_1^{m_1-1} \,\underline{\circ}\, (x_1^{n_1-1}\cdots x_{r-1}^{n_{r-1}-1})$ as a linear combination of monomials in $x_1^{n_1-1}\cdots x_r^{n_r-1}$.

Moreover, in [35, Proposition 3.3], Tasaka showed that all the matrices in the above product can be chosen with row and column indexing set being $S_{k,r}$, i.e., we have the following theorem.

Proposition 7.1.9 (Tasaka)**.** *The matrices $\mathcal{C}_{k,r}$ can be written as the product of $(r-1)$ square matrices*

$$\mathcal{C}_{k,r} = \prod_{i=2}^{r} \left(\delta\binom{m_1,\ldots,m_{r-i}}{n_1,\ldots,n_{r-i}} e\binom{m_{r-i+1},m_r}{n_{r-i+1},n_r} \right)_{\substack{(m_1,\ldots,m_r)\in S_{k,r} \\ (n_1,\ldots,n_r)\in S_{k,r}}}, \tag{7.1.6}$$

where the product is taken in the order $i = 2, 3, \ldots, r$.

7.2 Generalized matrices for any parities

Now instead of considering the matrix $\mathcal{C}_{k,r}$ corresponding to the totally odd motivic MZVs, we can also consider a matrix corresponding to motivic MZVs with any parity. Let $I \subseteq \mathrm{Total}_{k,r}$ be any indexing set of weight k and depth r. We define an $(|S_{k,r}| \times |I|)$-matrix $\mathcal{C}^I_{k,r}$ by

$$\mathcal{C}^I_{k,r} = \left(c\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r} \right)_{\substack{(m_1,\ldots,m_r)\in S_{k,r} \\ (n_1,\ldots,n_r)\in I}}, \tag{7.2.1}$$

where $c\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r}$ is as in (7.1.1). The same proof as for (7.1.5), using (7.1.4), yields the following proposition.

Proposition 7.2.1 (product formula)**.** *For any $I \subseteq \mathrm{Total}_{k,r}$, the $(|S_{k,r}|\times|I|)$ matrix $\mathcal{C}^I_{k,r}$ can be written as the product*

$$\begin{aligned} \mathcal{C}_{k,r} \quad = \quad & \left(\delta\binom{m_1,\ldots,m_{r-2}}{n_1,\ldots,n_{r-2}} e\binom{m_{r-1},m_r}{n_{r-1},n_r} \right)_{\substack{(m_1,\ldots,m_r)\in S_{k,r} \\ (n_1,\ldots,n_r)\in \mathrm{Total}_{k,r}}} \\ & \cdot \prod_{i=3}^{r-1} \left(\delta\binom{m_1,\ldots,m_{r-i}}{n_1,\ldots,n_{r-i}} e\binom{m_{r-i+1},\ldots,m_r}{n_{r-i+1},\ldots,n_r} \right)_{\substack{(m_1,\ldots,m_r)\in \mathrm{Total}_{k,r} \\ (n_1,\ldots,n_r)\in \mathrm{Total}_{k,r}}} \\ & \cdot \left(e\binom{m_1,\ldots,m_r}{n_1,\ldots,n_r} \right)_{\substack{(m_1,\ldots,m_r)\in \mathrm{Total}_{k,r} \\ (n_1,\ldots,n_r)\in I}}. \end{aligned}$$

Remark. For a general $I \subseteq \mathrm{Total}_{k,r}$, the middle matrices cannot be chosen with row and column indexing set being $S_{k,r}$.

Remark. Although the matrices $\mathcal{C}_{k,r}^{I}$ are defined here only in the case that $k \equiv r \pmod 2$, in the other case we can still define such matrices in a similar way using either the operator ∂_p or the linearized Ihara action.

7.3 Fake relations

7.3.1 Appearance of fake relations

The natural question to ask about this matrix $\mathcal{C}_{k,r}^{I}$ is whether the right annihilator of it always gives us a linear relation between depth-graded motivic MZVs of weight k and depth r with indices in $I \subseteq \mathrm{Total}_{k,r}$.

This is true when $r \leq 3$. But unfortunately, unlike the case when $I = S_{k,r}$ (conjectured by Conjecture 7.1.4), there are some elements in the right annihilator of $\mathcal{C}_{k,r}^{I}$ that do not give us a linear relation when $r \geq 4$.

Definition 7.3.1 (fake relation)**.** We call an element in the right annihilator of $\mathcal{C}_{k,r}^{I}$ that does not give a relation between depth-graded motivic MZVs of weight k and depth r with indices in I a fake relation.

As we mentioned above, Conjecture 7.1.4 predicts that there is no fake relation between totally odd motivic MZVs.

7.3.2 Examples

Starting from depth 4, there are elements in the right annihilators of the matrices $\mathcal{C}^I_{k,r}$ that do not give linear relations. We first give an example. Later we will show that these examples do not pass our criterion, so they correspond to fake relations.

Example 7.3.2. Let the weight k be 12, and let the depth r be 4. Then $S_{12,4} = \{(3,3,3,3)\}$. Take the index set I to be $\{(3,3,3,3),(1,1,8,2),(4,3,3,2),(3,6,1,2)\}$. Then the matrix $\mathcal{C}^I_{12,4}$ is the following 1×4 matrix

$$\mathcal{C}^I_{12,4} = (1,-6,-8,-2).$$

So the right annihilator is spanned by the following three column vectors

$$\begin{aligned} v_1 &= (6,1,0,0)^T, \\ v_2 &= (8,0,1,0)^T, \\ v_3 &= (2,0,0,1)^T. \end{aligned}$$

But all of them are fake relations, i.e., we have

$$\begin{aligned} 6\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,3,3,3) + \zeta^{\mathfrak{m}}_{\mathfrak{D}}(1,1,8,2) &\neq 0, \\ 8\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,3,3,3) + \zeta^{\mathfrak{m}}_{\mathfrak{D}}(4,3,3,2) &\neq 0, \\ 2\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,3,3,3) + \zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,6,1,2) &\neq 0. \end{aligned}$$

Before giving criteria for a relation to be fake, we will introduce two elements first. They will give us a criterion and a conjectural criterion respectively.

7.4 Depth 4 element $\overline{\mathbf{e}}$

Let $\mathfrak{g}$ denote the graded Lie algebra over $\mathbb{Q}$ freely generated by two elements e_0, e_1 of degree -1. It is the graded Lie algebra of the de Rham fundamental group ${}_0\Pi_1$ discussed Section 4.1.1. Its universal enveloping algebra is the tensor algebra

$$\mathcal{U}\mathfrak{g} = \bigoplus_{n\geq 0}(\mathbb{Q}e_0 \oplus \mathbb{Q}e_1)^{\otimes n}, \tag{7.4.1}$$

where the multiplication is given by the concatenation product. The motivic verison of the Drinfeld associator

$$\Phi^{\mathfrak{m}} = \sum_w wI^{\mathfrak{m}}(0;w;1) \in \mathcal{H}\langle\langle e_0, e_1\rangle\rangle,$$

where $I^{\mathfrak{m}}(0;w;1)$ for a word in e_0, e_1 is defined to be the corresponding motivic iterated integral with all e_i being replaced by i, defines a map from the graded dual of $\mathcal{H}$ to $\mathcal{U}\mathfrak{g}$

$$\begin{aligned} \Phi^{\mathfrak{m}} : \bigoplus_{k\geq 0}\mathcal{H}_k^{\vee} &\rightarrow \mathcal{U}\mathfrak{g}, \\ \psi &\mapsto \sum_w \psi(I^{\mathfrak{m}}(0;w;1))w. \end{aligned} \tag{7.4.2}$$

The image of this map is very difficult to describe, even conjecturally, since describing it is equivalent to describing all relations between motivic MZVs.

Remark. For example, by $\mathbf{I_2}$ and $\mathbf{I_3}$ in Section 4.1.3 and the formula (4.1.6) for the Drinfeld associator, the image of $\zeta^{\mathfrak{m}}(3)^{\vee}$ under the above map is $[e_0,[e_0,e_1]] + [e_1,[e_1,e_0]]$, which is equivalent to the relation $\zeta^{\mathfrak{m}}(3) = \zeta^{\mathfrak{m}}(1,2)$. In general, we do not know all the relations between motivic MZVs in high weight, which makes it impossible to write down the image of a high weight element.

To simplify the problem, let $\mathcal{L} = \mathcal{A}_{>0}/(\mathcal{A}_{>0})^2$ as before. The projection maps $\mathcal{H} \to \mathcal{A} \to \mathcal{L}$ induce a map $\bigoplus_{n\geq 0} \mathcal{L}_k^\vee \to \bigoplus_{k\geq 0} \mathcal{H}_k^\vee$, and we make the following definition for the image of $\bigoplus_{k\geq 0} \mathcal{L}_k^\vee$ in $\mathcal{U}\mathfrak{g}$.

Definition 7.4.1 (Set $\mathfrak{g}^{\mathfrak{m}}$ of motivic elements)**.** The set $\mathfrak{g}^{\mathfrak{m}}$ of motivic elements is the image of $\bigoplus_{k\geq 0} \mathcal{L}_k^\vee$ in $\mathcal{U}\mathfrak{g}$ under the map (7.4.2).

We have the following theorem about the structure of $\mathfrak{g}^{\mathfrak{m}}$ by Brown [4, Theorem 1.3].

Theorem 7.4.2 (Brown)**.** *The graded Lie algebra $\mathfrak{g}^{\mathfrak{m}}$ is non-canonically isomorphic to the free Lie algebra with one generator σ_{2i+1} in each degree $-(2i+1)$ for $i \geq 1$.*

Definition 7.4.3 (depth-graded Lie algebra)**.** The depth-graded Lie algebra is defined to be the associated bigraded Lie algebra $\mathfrak{dg}^{\mathfrak{m}}$ with the depth-graded piece

$$\mathfrak{dg}_r^{\mathfrak{m}} = \mathrm{gr}_r^{\mathfrak{D}} \mathfrak{g}^{\mathfrak{m}}. \tag{7.4.3}$$

It is the Lie algebra dual to the space of depth-graded motivic multiple zeta values modulo non-trivial products and $\zeta_{\mathfrak{D}}^{\mathfrak{m}}(2)$ (cf. [4, Section 1.3]).

Definition 7.4.4. Consider the isomorphism of $\mathbb{Q}$-vector spaces

$$\begin{aligned} \rho : \mathrm{gr}_r^{\mathfrak{D}} \mathcal{U}\mathfrak{g} &\to \mathbb{Q}[y_0, \ldots, y_r] \\ e_0^{a_0} e_1 e_0^{a_1} e_1 \cdots e_1 e_0^{a_r} &\mapsto y_0^{a_0} \cdots y_r^{a_r}. \end{aligned} \tag{7.4.4}$$

Let us denote the reduction map $\pi : \mathbb{Q}[y_0, y_1, \ldots, y_r] \to \mathbb{Q}[x_1, \ldots, x_r]$ which sends y_0 to 0 and y_i to x_i for $i = 1, \ldots, r$ by

$$\pi : f \mapsto \overline{f}.$$

Remark. Under the above isomorphism ρ and reduction π, the linearized action $\underline{\circ} : \mathcal{U}\mathfrak{g} \otimes_{\mathbb{Q}} \mathcal{U}\mathfrak{g} \to \mathcal{U}\mathfrak{g}$ induced from $U^{\mathrm{dR}} \times {}_0\Pi_1 \to {}_0\Pi_1$ becomes

$$\underline{\circ} : \mathbb{Q}[x_1, \ldots, x_r] \otimes_{\mathbb{Q}} \mathbb{Q}[x_1, \ldots, x_s] \to \mathbb{Q}[x_1, \ldots, x_{r+s}],$$

which is exactly the linearized Ihara action we defined in Definition 7.1.7 (cf. [4, Definition 2.1]).

Definition 7.4.5 (Reduced polynomial representation)**.** For any element $\xi \in \mathfrak{dg}^{\mathfrak{m}}$ of degree r we define $\overline{\rho}(\xi) := \overline{\rho(\xi)} \in \mathbb{Q}[x_1, \ldots, x_r]$ to be its reduced polynomial representation.

Studying $\mathfrak{dg}^{\mathfrak{m}}$ directly is very difficult. Instead, we try to study a subspace $\mathfrak{ls}$ of $\mathcal{U}\mathfrak{g}$ defined by the linearized double shuffle equations. (For any element in $\mathcal{U}\mathfrak{g}$, after replacing each word with its corresponding motivic iterated integral, that element satisfies the linearized double shuffle equations.) The linearized double shuffle equations are (cf. [4, Section 1.4]):

$$\begin{aligned} \zeta^{\mathfrak{m}}_{\mathfrak{D}}(w ⧢ w') &= 0 && \text{for all words } w, w' \text{ in } \{e_0, e_1\} \\ \zeta^{\mathfrak{m}}_{\mathfrak{D}}(y ⧢ y') &= 0 && \text{for all sequences of numbers } y, y' \text{ consisting of } \{1, 2, \ldots\} \\ \zeta^{\mathfrak{m}}_{\mathfrak{D}}(2n) &= 0 && \text{for all } n \geq 1, \end{aligned}$$

where the first shuffle product is for two words w, w', and the second shuffle product is shuffling the indices in $\zeta^{\mathfrak{m}}_{\mathfrak{D}}(n_1, \ldots, n_r)$. If w is a word in e^i, the symbol $\zeta^{\mathfrak{m}}(w)$ denotes the corresponding motivic iterated integral $I^{\mathfrak{m}}(0; w; 1)$. The space $\mathfrak{ls}$ satisfies

$$\mathfrak{dg}^{\mathfrak{m}} \subset \mathfrak{ls} \subset \mathcal{U}\mathfrak{g}. \tag{7.4.5}$$

Conjecturally (cf. [21, Section 8]), we should have $\mathfrak{dg}^{\mathfrak{m}} \cong \mathfrak{ls}$. But we will not discuss this conjecture in this paper.

In order to simplify the expressions in the following results, we consider their corresponding polynomial representations.

Definition 7.4.6 ($\mathbb{D}_r$)**.** Define $\mathbb{D}_r \subset \mathbb{Q}[x_1, \ldots, x_r]$ to be the space $\overline{\rho}(\mathfrak{ls}_r)$ in depth r. It is the space of polynomial solutions to the linearized double shuffle equation in depth r.

Now we are ready to define the element $\overline{\mathbf{e}}$.

Definition 7.4.7 (The element $\overline{\mathbf{e}}_f$)**.** Let $f \in \mathbb{Q}[x, y]$ be a restricted even period polynomial (see Definition 2.2.3). Define

$$f_0(x, y) = \frac{f(x, y)}{xy(x-y)} \quad \text{and} \quad f_1(x, y) = \frac{f(x, y)}{xy}. \tag{7.4.6}$$

Note that $f_0, f_1 \in \mathbb{Q}[x, y]$. The element $\mathbf{e}_f \in \mathbb{Q}[y_0, y_1, y_2, y_3, y_4]$ is defined to be

$$\mathbf{e}_f = \sum_{i=0}^{4} \big(f_1(y_{\sigma^i(4)} - y_{\sigma^i(3)}, y_{\sigma^i(2)} - y_{\sigma^i(1)}) + (y_{\sigma^i(0)} - y_{\sigma^i(1)}) f_0(y_{\sigma^i(2)} - y_{\sigma^i(3)}, y_{\sigma^i(4)} - y_{\sigma^i(3)})\big), \tag{7.4.7}$$

where $\sigma = (0\ 1\ 2\ 3\ 4)$ is a cyclic permutation of the 5 elements $\{0, 1, 2, 3, 4\}$. We let $\overline{\mathbf{e}}_f := \pi(\mathbf{e}_f) \in \mathbb{Q}[x_1, \ldots, x_4]$ be the reduction of $\mathbf{e}_f$.

Theorem 7.4.8. *The reduced polynomial $\overline{\mathbf{e}}_f$ satisfies the linearized double shuffle equations. In particular, we get an injective linear map*

$$\overline{\mathbf{e}} : \mathcal{S} \to \mathbb{D}_4, \quad f \mapsto \overline{\mathbf{e}}_f := \overline{\mathbf{e}}_{r_f^-, 0} \tag{7.4.8}$$

where $\mathcal{S} = \bigoplus_{k \geq 12} \mathcal{S}_k$ is the space of cusp forms.

Remark. For a general restricted even period polynomial f, we know that the element $\overline{\mathbf{e}}_f$ lies in $\overline{\rho}(\mathfrak{ls}_4)$, but we do not know whether it lies in $\overline{\rho}(\mathfrak{dg}_4^{\mathfrak{m}})$, i.e., it has not been shown to be motivic.

7.5 Depth 4 elements $\mathfrak{c}$

The other element $\mathfrak{c}$ we want to define in this section lies in the space $\mathfrak{dg}_4^{\mathfrak{m}}$, so it is automatically motivic. But as we will see, its polynomial representation is much more complicated than $\overline{\mathbf{e}}$ defined above. The starting point of this section is the following theorem of Brown [7, Section 1.1].

Theorem 7.5.1 (Brown)**.** *There is a morphism of Lie algebras*

$$i_0 : \mathfrak{g}^{\mathfrak{m}} \to \mathrm{Der}^1\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$$

where $\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ *is the free Lie algebra on two generators* $\mathbf{x}_0, \mathbf{x}_1$*, and* $\mathrm{Der}^1\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ *denotes the Lie algebra of derivations that send* $\mathbf{x}_1$ *to* 0*. This morphism factors through an injective morphism of Lie algberas*

$$i : \mathfrak{g}^{\mathfrak{m}} \to \mathbb{L}(\mathbf{x}_0, \mathbf{x}_1),$$

where the morphism i_0 *maps* $\sigma \in \mathfrak{g}^{\mathfrak{m}}$ *to the derivation which satisfies*

$$\mathbf{x}_0 \mapsto [i(\sigma), \mathbf{x}_0] \qquad \text{and} \qquad \mathbf{x}_1 \mapsto 0.$$

Definition 7.5.2 (Depth filtration on $\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$)**.** The depth filtration $\mathfrak{D}^r\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ is the decreasing filtration on $\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ such that $\mathfrak{D}^r\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ consists of $\mathbb{Q}$-linear combinations of Lie brackets of $\mathbf{x}_0$ and $\mathbf{x}_1$ with at least r $\mathbf{x}_1$'s.

As before, there are polynomial representations of the elements in $\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ given by the following injective map

$$\begin{aligned} \overline{\rho}: \qquad \mathbb{L}(\mathbf{x}_0, \mathbf{x}_1) &\to \mathbb{Q}[x_1, \ldots, x_r] \\ \mathbf{x}_0^{i_0}\mathbf{x}_1\mathbf{x}_0^{i_1}\mathbf{x}_1 \cdots \mathbf{x}_1\mathbf{x}_0^{i_r} &\mapsto x_1^{i_1}x_2^{i_2}\cdots x_r^{i_r}. \end{aligned} \tag{7.5.1}$$

In [7], Brown found a canonical solution up to depth 3 for the linearized double shuffle equations (a solution for the linearized double shuffle equations modulo depth ≥ 4 parts), and used it to construct a depth 4 element $\mathfrak{c}$ that we want to discuss here. As opposed to the case of $\overline{\mathbf{e}}$, which is not known to be motivic, Brown showed that this depth 4 element $\mathfrak{c}$ is actually motivic.

Definition 7.5.3. For $n \geq -1$, define rational functions in x_1, x_2, x_3 by

$$\xi^{(1)}_{2n+1} = x_1^{2n} \tag{7.5.2}$$

$$\xi^{(2)}_{2n+1} = \{s^{(1)}, x_1^{2n}\} \tag{7.5.3}$$

$$\xi^{(3)}_{2n+1} = \{s^{(2)}, x_1^{2n}\} + \frac{1}{2}\{s^{(1)}, \{s^{(1)}, x_1^{2n}\}\}, \tag{7.5.4}$$

where curly brackets denote the linearized Ihara bracket given by $\{f, g\} = f \,\underline{\circ}\, g - g \,\underline{\circ}\, f$ with the same formula in Definition 7.1.7 applying to the rational functions, and

$$s^{(1)} = \frac{1}{2x_1}, \qquad s^{(2)} = \frac{1}{12}\left(\frac{1}{x_1x_2} + \frac{1}{x_2(x_1 - x_2)}\right). \tag{7.5.5}$$

Proposition 7.5.4. *Let $n \geq -1$. The elements*

$$(\xi^{(1)}_{2n+1}, \xi^{(2)}_{2n+1}, \xi^{(3)}_{2n+1})$$

satisfy the double shuffle equation in depths 2 and 3.

Remark. Here the double shuffle equation in depths 2 and 3 means the following four equations for $(f^{(1)}, f^{(2)}, f^{(3)}) \in \mathbb{Q}(x_1) \oplus \mathbb{Q}(x_1, x_2) \oplus \mathbb{Q}(x_1, x_2, x_3)$:

$$\begin{aligned} f^{(2)}(x_1, x_{12}) + f^{(2)}(x_2, x_{12}) &= 0, \\ f^{(3)}(x_1, x_{12}, x_{123}) + f^{(3)}(x_2, x_{12}, x_{123}) + f^{(3)}(x_2, x_{23}, x_{123}) &= 0, \end{aligned}$$

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

where x_{ij} stands for $x_i + x_j$ and x_{ijk} stands for $x_i + x_j + x_k$.

Now we can use this above polar solution of double shuffle equations to construct a polynomial solution of the linearized double shuffle equations.

Definition 7.5.5. For any $n \geq 1$, define the element $\sigma^c_{2n+1} \in \mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)/\mathfrak{D}^4\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)$ as follows

$$\rho((\sigma^c_{2n+1})^{(1)}) = \xi^{(1)}_{2n+1} \quad \text{for } n \geq 1, \tag{7.5.6}$$

$$\rho((\sigma^c_{2n+1})^{(2)}) = \xi^{(2)}_{2n+1} \quad \text{for } n \geq 1, \tag{7.5.7}$$

$$\rho((\sigma^c_{3})^{(3)}) = 0, \tag{7.5.8}$$

$$\rho((\sigma^c_{2n+1})^{(3)}) = \xi^{(3)}_{2n+1} + \sum_{\substack{a+b=n \\ a,b \geq 1}} \frac{B_{2a}B_{2b}}{B_{2n}} \binom{2n}{2a} \frac{1}{24b} \{x_1^{2a}, \{x_1^{2b}, x_1^{-2}\}\} \quad \text{for } n \geq 2. \tag{7.5.9}$$

For future use, define

$$z_3 = \frac{4}{3} + \frac{x_1}{x_3 - x_2} + \frac{x_3}{x_1 - x_2} + \frac{x_3 - x_2}{x_1} + \frac{x_1 - x_2}{x_3}, \tag{7.5.10}$$

which is exactly the polar part of (7.5.9) for $n = 1$.

Brown showed that the element σ^c_{2n+1} defined above are motivic, i.e., we have

Theorem 7.5.6. *The elements σ^c_{2n+1} are in the image of the map*

$$i_0 : \mathfrak{dg}^{\mathfrak{m}}_1 \oplus \mathfrak{dg}^{\mathfrak{m}}_2 \oplus \mathfrak{dg}^{\mathfrak{m}}_3 \to \mathbb{L}(\mathbf{x}_0, \mathbf{x}_1)/\mathfrak{D}^4\mathbb{L}(\mathbf{x}_0, \mathbf{x}_1).$$

Remark. The canonical elements σ^c_{2n+1} define maps from motivic MZVs in depth $r \leq 3$ and odd weight to rational numbers given by

$$(\sigma^c_{2n+1})^{(r)}\zeta^{\mathfrak{m}}(n_1, \ldots, n_r) = \text{ coefficient of } x_1^{n_1-1} \cdots x_r^{n_r-1} \text{ in } \rho((\sigma^c_{2n+1})^{(r)}),$$

where $1 \leq r \leq 3$ and $2n + 1 = n_1 + \cdots + n_r$.

Definition 7.5.7. Let $f(x_1, x_2) = \sum_{i,j} \lambda_{i,j} x_1^{2i} x_2^{2j}$ be a restricted even period polynomial of weight k. The element $\mathfrak{c}_f \in \mathfrak{dg}^{\mathfrak{m}}_{k,4}$ is defined to be

$$\mathfrak{c}_f = \left(\sum_{i<j} \lambda_{i,j} \{\sigma^c_{2i+1}, \sigma^c_{2j+1}\} \right)^{(4)}. \tag{7.5.11}$$

In [7], Brown gave the following explicit formula for the depth 4 element $\mathfrak{c}_f$.

Theorem 7.5.8. *Let $f(x_1, x_2) = \sum_{i,j} \lambda_{i,j} x_1^{2i} x_2^{2j}$ be a restricted even period polynomial of weight k. Since $\lambda_{i,j} = -\lambda_{j,i}$, this f gives rise to a relation of the form*

$$\sum_{i<j} \lambda_{i,j} \{(\sigma^c_{2i+1})^{(1)}, (\sigma^c_{2j+1})^{(1)}\} = 0 \text{ in } \mathfrak{dg}^{\mathfrak{m}}_{k,2}.$$

Then the image of the element $\mathfrak{c}_f \in \mathfrak{dg}_{k,4}$ *in* $\mathbb{Q}[x_1, x_2, x_3, x_4]$ *is*

$$\begin{aligned}\overline{\rho}(\mathfrak{c}_f) &= \sum_{i,a,b} \lambda_{i,a+b} \frac{B_{2a}B_{2b}}{B_{2a+2b}} \binom{2a+2b}{2a} \frac{1}{24b} \{x_1^{2i}, \{x_1^{2a}, \{x_1^{2b}, x_1^{-2}\}\}\} \\ &\quad -3 \sum_i \lambda_{i,2} \{x_1^{2i}, z_3\}, \end{aligned} \tag{7.5.12}$$

where z_3 *is defined in (7.5.10).*

7.6 A conjectural connection between $\overline{\mathbf{e}}_f$ and $\mathfrak{c}_f$

In [7], Brown asked the question of what the relation between those two depth 4 elements $\mathfrak{c}_f$ and $\overline{\mathbf{e}}_f$ is. In this section, we identify $\mathfrak{c}_f$ with its polynomial representation $\overline{\rho}(\mathfrak{c}_f)$. If f is a cusp form instead of a restricted even period polynomial, $\mathfrak{c}_f$ and $\overline{\mathbf{e}}_f$ stands for $\mathfrak{c}_{r_f^-,0}$ and $\overline{\mathbf{e}}_{r_f^-,0}$ respectively.

Recall that the $((m_1, \ldots, m_r), (n_1, \ldots, n_r))$th entry of the matrix $\mathcal{C}_{k,r}^{\mathrm{Total}_{k,r}}$ is the coefficient of $x_1^{n_1-1} \cdots x_r^{n_r-1}$ in

$$x_1^{m_1-1} \,\underline{\circ}\, (\cdots x_1^{m_{r-2}-1} \,\underline{\circ}\, (x_1^{m_{r-1}-1} \,\underline{\circ}\, x_1^{m_r-1}) \cdots),$$

which is exactly the coefficient of $x_1^{n_1-1} \cdots x_r^{n_r-1}$ in

$$\sigma_{m_1}^{(1)} \,\underline{\circ}\, (\cdots \sigma_{m_{r-2}}^{(1)} \,\underline{\circ}\, (\sigma_{m_{r-1}}^{(1)} \,\underline{\circ}\, \sigma_{m_r}^{(1)}) \cdots).$$

Here $\sigma_i^{(i)}$ stands for $(\sigma_i^c)^{(1)}$.

We can use an extended matrix $\widetilde{\mathcal{C}}_{k,4}^{\mathrm{Total}_{k,4}}$ to state the conjectural connection between $\mathfrak{c}_f$ and $\overline{\mathbf{e}}_f$.

Definition 7.6.1 (extended matrix $\widetilde{\mathcal{C}}_{k,4}^{\mathrm{Total}_{k,4}}$)**.** Define $\widetilde{\mathcal{C}}_{k,4}^{\mathrm{Total}_{k,4}}$ to be the following extended matrix, where the minor containing only the first $|S_{k,r}|$ rows is the original

$\mathcal{C}_{k,4}^{\mathrm{Total}_{k,4}}$:

$$\left(\begin{array}{c||c} \text{Rows} \diagdown \text{Columns} & \mathrm{Total}_{k,4} \\ \hline\hline \sigma_{m_1}^{(1)} \mathbin{\underline{\circ}} (\sigma_{m_2}^{(1)} \mathbin{\underline{\circ}} (\sigma_{m_3}^{(1)} \mathbin{\underline{\circ}} \sigma_{m_4}^{(1)})) & \text{coeff. of } x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1} \\ \hline \mathfrak{c}_f & \text{coeff. of } x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1} \end{array}\right)_{\substack{(m_1,m_2,m_3,m_4)\in S_{k,4} \\ f\in\mathfrak{B} \\ (n_1,n_2,n_3,n_4)\in \mathrm{Total}_{k,4}}} \tag{7.6.1}$$

Here f runs through a basis $\mathfrak{B}$ of $\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ consisting of normalized eigenforms.

Remark. This matrix $\widetilde{\mathcal{C}}_{k,4}^{\mathrm{Total}_{k,4}}$ has exactly $\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ more rows than $\mathcal{C}_{k,4}^{\mathrm{Total}_{k,4}}$.

The following conjecture tells us the relationship between the elements $\overline{\mathbf{e}}_f$ and $\mathfrak{c}_f$ for any $f \in \mathbf{W}^{-,0}(\mathbb{Q})$.

Conjecture 7.6.2 (Relation between $\overline{\mathbf{e}}$ and $\mathfrak{c}$)**.** *We write the matrix $\widetilde{\mathcal{C}}_{k,4}^{\mathrm{Total}_{k,4}}$ as a block matrix with 4 blocks in the following way.*

$$\widetilde{\mathcal{C}}_{k,4}^{\mathrm{Total}_{k,4}} = \left(\begin{array}{c||c|c} \textit{Rows} \diagdown \textit{Columns} & S_{k,4} & \mathrm{Total}_{k,4} \setminus S_{k,4} \\ \hline\hline \sigma_{m_1}^{(1)} \mathbin{\underline{\circ}} (\sigma_{m_2}^{(1)} \mathbin{\underline{\circ}} (\sigma_{m_3}^{(1)} \mathbin{\underline{\circ}} \sigma_{m_4}^{(1)})) & \mathcal{C}_{k,4} & B \\ \hline \mathfrak{c}_f & C & D \end{array}\right)_{\substack{(m_1,m_2,m_3,m_4)\in S_{k,4} \\ f\in\mathfrak{B} \\ (n_1,n_2,n_3,n_4)\in \mathrm{Total}_{k,4}}}$$

By elementary row and column operations of the second type (adding a multiple of one row or column to another), we transform it into the form

$$\left(\begin{array}{c||c|c} \textit{Rows} \diagdown \textit{Columns} & S_{k,4} & \mathrm{Total}_{k,4} \setminus S_{k,4} \\ \hline\hline \sigma_{m_1}^{(1)} \mathbin{\underline{\circ}} (\sigma_{m_2}^{(1)} \mathbin{\underline{\circ}} (\sigma_{m_3}^{(1)} \mathbin{\underline{\circ}} \sigma_{m_4}^{(1)})) & \mathcal{C}_{k,4} & 0 \\ \hline \mathfrak{c}_f & 0 & E \end{array}\right)_{\substack{(m_1,m_2,m_3,m_4)\in S_{k,4} \\ f\in\mathfrak{B} \\ (n_1,n_2,n_3,n_4)\in \mathrm{Total}_{k,4}}}$$

Then for each row E_f of E corresponding to $f \in \mathfrak{B}$, we have $E_f = \lambda_f \cdot \overline{\mathbf{e}}_f$ with

$$\lambda_f = -\frac{1}{4} \cdot \frac{\textit{2nd period of the eigenform}}{\textit{0th period of the eigenform}}, \tag{7.6.2}$$

where nth period of a cusp form of weight k is defined to be the coefficient of the $x^n y^{k-2-n}$ *term in the period polynomial* $r_f(x, y)$.

Remark. Since $\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ has a basis consisting of cusp forms with rational coefficients, by taking the corresponding rational basis for $\mathbf{W}_k^{-,0}(\mathbb{C})$ via the Eichler-Shimura-Manin correspondence, we can arrange that the last $|\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))|$ rows have entries in $\mathbb{Q}$. But if we do that, the connection between $\overline{\mathbf{e}}_f$ and $\mathfrak{c}_f$ is not clear anymore.

Example 7.6.3. In weight 12, for any nonzero restricted even period polynomial $f \in \mathbf{W}_{12}^{-,0}$, we have

$$\lambda_f = -\frac{1}{4} \cdot \frac{-1}{\frac{36}{691}} = \frac{691}{144}.$$

From the computation described in Conjecture 7.6.2, we also get

$$E_f = \frac{691}{144} \overline{\mathbf{e}}_f.$$

Similarly, in weight 16, for any nonzero restricted even period polynomial $f \in \mathbf{W}_{16}^{-,0}$, we have

$$\lambda_f = -\frac{1}{4} \cdot \frac{-1}{\frac{180}{3617}} = \frac{3617}{720}.$$

From the computation described in Conjecture 7.6.2, we also get

$$E_f = \frac{3617}{720} \overline{\mathbf{e}}_f.$$

Remark. Conjecture 7.6.2 can also explain the appearance of the irregular primes 691, 3617, and so on. This is related to the extensive work on the Galois side originated by Ihara [20].

7.7 Two criteria for the appearance of fake relations in depth 4

7.7.1 A criterion from $\mathfrak{c}$

Throughout this section, we will simply write σ_i^c as σ_i. The element $\mathfrak{c}$ defined in Definition 7.5.7 gives us the following criterion for the appearance of fake relations in depth 4.

Proposition 7.7.1 (A criterion from $\mathfrak{c}$)**.** *Let k be an even integer, and let $I \subset \mathrm{Total}_{k,4}$ be any indexing set. A relation*

$$\sum_{(n_1,n_2,n_3,n_4)\in I} a_{(n_1,n_2,n_3,n_4)}\zeta_{\mathfrak{D}}^{\mathfrak{m}}(n_1,n_2,n_3,n_4)=0$$

coming from an element $(a_{(n_1,n_2,n_3,n_4)})_{(n_1,n_2,n_3,n_4)\in I}$ in the right annihilator of $\mathcal{C}_{k,4}^I$ is not a fake relation if and only if the corresponding linear combination

$$\sum_{(n_1,n_2,n_3,n_4)\in I} a_{(n_1,n_2,n_3,n_4)}c^f_{(n_1,n_2,n_3,n_4)}$$

of the coefficient $c^f_{(n_1,n_2,n_3,n_4)}$ of $x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1}$ with $(n_1,n_2,n_3,n_4)\in I$ in $\mathfrak{c}_f$ vanishes for all $f\in \mathbf{W}_N^{-,0}(\mathbb{Q})$.

Proof. We first look at the image of MZV of depth 4 under $\phi:\mathcal{H}\to\mathcal{U}$. For any $(n_1,n_2,n_3,n_4)\in \mathrm{Total}_{k,4}$, we have

$$\begin{aligned}\phi(\zeta^{\mathfrak{m}}(n_1,n_2,n_3,n_4)) &= \sum_{\substack{i+j+l+m=k\\ i,j,l,m\geq 3:\text{odd}}} a_{i,j,k,l}f_if_jf_kf_l+\sum_{\substack{i+j+2l=k\\ i,j\geq 3:\text{odd}\\ l\geq 1}} a_{i,j,2l}f_if_jf_{2l}\\ &\quad+\sum_{\substack{i+j=k\\ i,j\geq 3:\text{odd}}} a_{i,j}f_if_j+a_kf_k,\end{aligned}$$

where the coefficient $a_{i,j,l,m}$ in the motivic depth 4 part is computed by the coefficient of $x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1}$ in

$$\sigma_i^{(1)} \underline{\circ} (\sigma_j^{(1)} \underline{\circ} (\sigma_l^{(1)} \underline{\circ} \sigma_m^{(1)})).$$

Moreover, the coefficient $a_{i,j,2l}$ in the motivic depth 3 part is computed by the coefficient of $x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1}$ in

$$(\sigma_i \underline{\circ} (\sigma_j \underline{\circ} \tau_{2l}))^{(4)},$$

where τ_{2l} is the even weight analogue of σ_{2l+1} (the canonical solution of the linearized double shuffle equations for even weight $2l$) with the normalization

$$\tau_{2l}\zeta^{\mathfrak{m}}(2l) = 1.$$

See [7], but note that our normalization is a little different from it.

Now for any l and the coefficients λ_{ij} of a restricted even period polynomial of weight $k-2l$, we have

$$\sum_{i,j} \lambda_{ij}(\sigma_i \underline{\circ} (\sigma_j \underline{\circ} \tau_{2l}))^{(4)} = \left(\left(\sum \lambda_{ij}\sigma_i \underline{\circ} \sigma_j\right) \underline{\circ} \tau_{2l}\right)^{(4)} = 0,$$

by the period polynomial relations in depth 2 (cf. [16], [34]) and the parity result in depth 3 (cf. [4], [21]), we have

$$\left(\sum_{i,j} \lambda_{ij}\sigma_i \underline{\circ} \sigma_j\right)^{(2)} = \left(\sum_{i,j} \lambda_{ij}\sigma_i \underline{\circ} \sigma_j\right)^{(3)} = 0.$$

Therefore, by the period polynomial relations in depth 2, we know that the motivic depth 3 part can be recovered by the image of some linear combination of MZVs of depth 3:

$$\phi\Big(\sum_{i+j+2l=k} b_{i,j,2l}\zeta^{\mathfrak{m}}(i,j)\zeta^{\mathfrak{m}}(2l)\Big).$$

Therefore, modulo lower depth, the motivic depth 3 part does not appear in the image of ϕ (it is also clear that we do not have a depth 1 part), i.e., we have

$$\phi\Big(\zeta^{\mathfrak{m}}(n_1,n_2,n_3,n_4) - (\text{depth} \le 3)\Big) = \sum_{\substack{i+j+l+m=k\\ i,j,l,m\ge 3 \text{ odd}}} a_{i,j,l,m} f_i f_j f_l f_m + \sum_{\substack{i+j=k\\ i,j\ge 3 \text{ odd}}} b_{i,j} f_i f_j.$$

Every element $(v_{(n_1,n_2,n_3,n_4)})^T$ in the right annihilator of $\mathcal{C}^I_{k,4}$ would give us

$$\phi\Bigg(\sum_{(n_1,n_2,n_3,n_4)\in I} v_{(n_1,n_2,n_3,n_4)}\zeta^{\mathfrak{m}}(n_1,n_2,n_3,n_4) - (\text{depth} \le 3)\Bigg) = \sum_{\substack{i+j=k\\ i,j\ge 3 \text{ odd}}} c_{i,j} f_i f_j,$$

for some $c_{i,j} \in \mathbb{Q}$, since by definition, element in the right annihilator of $\mathcal{C}^I_{k,4}$ would annihilate the depth 4 part. The motivic depth 2 part on the righthand side is the image of a depth 2 motivic MZV if and only if

$$(c_{3,k-3}, c_{5,k-5}, \dots, c_{k-3,3}) \perp (\lambda_{3,k-3}, \lambda_{5,k-5}, \dots, \lambda_{k-3,3})$$

under the usual inner product in the Euclidean space for all $\sum_{i,j} \lambda_{i,j} x^{i-1} y^{j-1} \in \mathbf{W}_k^{-,0}(\mathbb{Q})$ (cf. [34]). Therefore, the part of the motivic depth 2 part which is not coming from an image of some depth 2 motivic MZV is exactly detected by the

$$\sum_{\substack{i+j=k\\ i,j\ge 3 \text{ odd}}} \lambda_{i,j} f_i f_j$$

for $\sum_{i,j} \lambda_{i,j} x^{i-1} y^{j-1} \in \mathbf{W}_k^{-,0}(\mathbb{Q})$, which is equivalent to the corresponding linear combination of the coefficients of $x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1}$ with $(n_1,n_2,n_3,n_4) \in I$ in the coefficient of $\mathfrak{c}_f$ for all $f \in \mathbf{W}_k^{-,0}(\mathbb{Q})$. Hence we have proved the statement. $\square$

7.7.2 A conjectural criterion coming from $\overline{\mathbf{e}}$

From the conjectural connection between $\mathfrak{c}$ and $\overline{\mathbf{e}}$ in Conjecture 7.6.2, we obtain the following conjectural criterion.

Conjecture 7.7.2 (A conjectural criterion from $\overline{\mathbf{e}}$). *Let k be an even integer, and let $I \subset \mathrm{Total}_{k,4}$ be any indexing set. A relation*

$$\sum_{(n_1,n_2,n_3,n_4)\in I} a_{(n_1,n_2,n_3,n_4)} \zeta_{\mathfrak{D}}^{\mathfrak{m}}(n_1,n_2,n_3,n_4) = 0$$

coming from an element $(a_{(n_1,n_2,n_3,n_4)})_{(n_1,n_2,n_3,n_4)\in I}$ in the right annihilator of $\mathcal{C}_{k,4}^{I}$ is not a fake relation if and only if the corresponding linear combination

$$\sum_{(n_1,n_2,n_3,n_4)\in I} a_{(n_1,n_2,n_3,n_4)} e^{f}_{(n_1,n_2,n_3,n_4)}$$

of the coefficient $e^{f}_{(n_1,n_2,n_3,n_4)}$ of $x_1^{n_1-1}x_2^{n_2-1}x_3^{n_3-1}x_4^{n_4-1}$ with $(n_1,n_2,n_3,n_4)\in I$ in $\overline{\mathbf{e}}_f$ vanishes for all $f \in \mathbf{W}_N^{-,0}(\mathbb{Q})$.

The first criterion from Proposition 7.7.1 is a genuine criterion, but it is hard to apply because the element $\mathfrak{c}$ is difficult to compute. The second one from Conjecture 7.7.2 is a conjectural criterion, but it is easy to use because the element $\overline{\mathbf{e}}$ is easy to compute.

Remark. In Proposition 7.7.1 and Conjecture 7.7.2, we can change the statement from "for all $f \in \mathbf{W}_k^{-,0}(\mathbb{Q})$" to "for all f in a basis of $\mathbf{W}_k^{-,0}(\mathbb{Q})$".

7.7.3 Examples of genuine relations and fake relations

Example 7.7.3. The following three relations are the fake relations we listed in Example 7.3.2:

$$\begin{aligned} 6\zeta_{\mathfrak{D}}^{\mathfrak{m}}(3,3,3,3)+\zeta_{\mathfrak{D}}^{\mathfrak{m}}(1,1,8,2) &\neq 0, \\ 8\zeta_{\mathfrak{D}}^{\mathfrak{m}}(3,3,3,3)+\zeta_{\mathfrak{D}}^{\mathfrak{m}}(4,3,3,2) &\neq 0, \\ 2\zeta_{\mathfrak{D}}^{\mathfrak{m}}(3,3,3,3)+\zeta_{\mathfrak{D}}^{\mathfrak{m}}(3,6,1,2) &\neq 0. \end{aligned}$$

Now let us see how to use the conjectural criterion for $\overline{\mathbf{e}}$ to get the conclusion that these are fake relations. Since $\dim \mathcal{S}_{12}(\mathrm{SL}_2(\mathbb{Z}))=1$, there is only one restricted even period polynomial up to a scalar. Take $f(x,y)=x^8y^2-3x^6y^4+3x^4y^6-x^2y^8$. From [4, Example 8.3], we have

$$\overline{\mathbf{e}}_f = 0x_1^2x_2^2x_3^2x_4^2 + x_3^7x_4 - 116x_1^3x_2^2x_3^2x_4 - 57x_1^2x_2^5x_4 + \cdots .$$

Here we only list those 4 terms since

$$I=\{(3,3,3,3),(1,1,8,2),(4,3,3,2),(3,6,1,2)\}.$$

Now since

$$\begin{aligned} 6\cdot 0+1\cdot 1 &\neq 0, \\ 8\cdot 0+1\cdot(-116) &\neq 0, \\ 2\cdot 0+1\cdot(-57) &\neq 0, \end{aligned}$$

they are all fake relations by our conjectural criterion from $\overline{\mathbf{e}}$.

But for the element $(8, 15, -21, 43)^T$ in the right annihilator of $\mathcal{C}^I_{12,4}$, we have

$$8 \cdot 0 + 15 \cdot 1 - 21 \cdot (-116) + 43 \cdot (-57) = 0.$$

Therefore, the relation

$$8\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,3,3,3) + 15\zeta^{\mathfrak{m}}_{\mathfrak{D}}(1,1,8,2) - 21\zeta^{\mathfrak{m}}_{\mathfrak{D}}(4,3,3,2) + 43\zeta^{\mathfrak{m}}_{\mathfrak{D}}(3,6,1,2) = 0$$

is a genuine relation modulo lower depth. A similar but more complicated computation can also be done using Proposition 7.7.1, but we do not describe it in detail here.

CHAPTER 8

Multiple Zeta Values of Depth 2 and Level N

In this chapter, we will introduce the notion of multiple zeta values of level N. After introducing Glanois' result about derivation operators, we will define the matrix $\mathcal{C}_{k,2}^N$ and $\mathcal{D}_{k,2}^N$ for $N = 2, 3$. We will prove two results about the connections with Hecke operators and the spaces of newforms. At the end, we will give a conjectural generalization of the Eichler-Shimura-Manin correspondence to the space of newforms of levels 2 and 3. The results in this chapter can be found in [25].

8.1 MZVs of level N and their motivic setting

Multiple zeta values of level N are defined by

$$\zeta\binom{n_1, \cdots, n_r}{\varepsilon_1, \cdots, \varepsilon_r} := \sum_{0<k_1<\cdots<k_r} \frac{\varepsilon_1^{k_1} \cdots \varepsilon_r^{k_r}}{k_1^{n_1} \cdots k_r^{n_r}}, \quad \varepsilon_i \in \mu_N, \ (n_r, \varepsilon_r) \neq (1, 1). \tag{8.1.1}$$

As in the setting of MZVs case, the weight is $n_1 + \cdots + n_r$, and the depth is r. Denote by $\mathcal{Z}^N$ the $\mathbb{Q}$-vector space spanned by these multiple zeta values at arguments $n_i \in \mathbb{Z}_{\geq 1}$, $\varepsilon_i \in \mu_N$. There exist motivic versions of those multiple zeta values, denoted by $\zeta^{\mathfrak{m}}$, which span the $\mathbb{Q}$-vector space of motivic multiple zeta values of level N, denoted by $\mathcal{H}^N$. There is a surjective homomorphism called the period map as in the MZV case, conjectured also to be an isomorphism (a variant of Grothendieck's period conjecture):

$$\begin{aligned} per : \mathcal{H}^N &\rightarrow \mathcal{Z}^N \\ \zeta^{\mathfrak{m}}(\cdot) &\mapsto \zeta(\cdot). \end{aligned} \tag{8.1.2}$$

Let ${}_0\Pi_1^{(N)}$ denote the de Rham fundamental group of $\mathbb{P}^1 \setminus \{0, \mu_N, \infty\}$. Its affine ring of regular functions is the graded algebra for the shuffle product:

$$\mathcal{O}({}_0\Pi_1^{(N)}) \cong \mathbb{Q}\langle e^0, (e^\eta)_{\eta\in\mu_N}\rangle. \tag{8.1.3}$$

Let $\mathcal{MT}_N$ be the Tannakian category of the mixed Tate motives. Denote by $\mathcal{MT}'_N$ the full Tannakian subcategory of $\mathcal{MT}_N$ generated by the motivic fundamental groupoid of $\mathbb{P}^1 \setminus \{0, \mu_N, \infty\}$. Denote also by $\mathcal{G}_N = \mathbb{G}_m \ltimes \mathcal{U}_N$ its Galois group defined over $\mathbb{Q}$, $\mathcal{A}^N = \mathcal{O}(\mathcal{U}_N)$ its fundamental Hopf algebra and $\mathcal{L}^N := \mathcal{A}^N_{>0}/(\mathcal{A}^N_{>0})^2$ the Lie coalgebra of indecomposable elements.

8.2 The operators D_p and ∂_p^η

In this section, we will define the operators D_p and ∂_p^η, which generalize D_p and ∂_p in Sections 4.3 and 7.1.1. For integers $N, p \geq 1$, Glanois [15] defined derivation operators

$$D_p : \mathcal{H}^N \rightarrow \mathcal{L}_r^N \otimes \mathcal{H}^N \tag{8.2.1}$$

by using the coaction Δ for motivic iterated integrals defined by Goncharov [18] and extended by Brown [6]. In [15, Lemma 2.8], Glanois gave the following explicit formula for the operator D_p.

Proposition 8.2.1 (Glanois). *For any integers $N, p, r \geq 1$, we have*

$$\begin{aligned}
D_p : \mathrm{gr}_r^{\mathfrak{D}} \mathcal{H}^N &\to \mathrm{gr}_1^{\mathfrak{D}} \mathcal{L}_p^N \otimes \mathrm{gr}_{r-1}^{\mathfrak{D}} \mathcal{H}^N \\
\zeta^{\mathfrak{m}}\binom{n_1, \ldots, n_r}{\varepsilon_1, \ldots, \varepsilon_r} &\mapsto \delta_{p=n_1} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_1} \otimes \zeta^{\mathfrak{m}}\binom{n_2, \ldots}{\varepsilon_2, \ldots} \\
&\quad + \sum_{i=2}^{r-1} \delta_{n_i \leq p < n_i + n_{i-1} - 1} (-1)^{p-n_i} \binom{p-1}{p-n_i} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_i} \\
&\qquad \otimes \zeta^{\mathfrak{m}}\binom{\ldots, n_i + n_{i-1} - p, \ldots}{\ldots, \varepsilon_{i-1}\varepsilon_i, \ldots} \\
&\quad + \sum_{i=1}^{r-1} \delta_{n_i \leq p < n_i + n_{i+1} - 1} (-1)^{n_i} \binom{p-1}{p-n_i} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_i^{-1}} \\
&\qquad \otimes \zeta^{\mathfrak{m}}\binom{\ldots, n_i + n_{i+1} - p, \ldots}{\ldots, \varepsilon_{i+1}\varepsilon_i, \ldots} \\
&\quad + \sum_{i=2}^{r-1} \delta_{\substack{p = n_i + n_{i-1} - 1 \\ \varepsilon_{i-1}\varepsilon_i \neq 1}} \left((-1)^{n_i} \binom{p-1}{n_i - 1} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_{i-1}^{-1}} \right. \\
&\qquad \left. + (-1)^{n_{i-1}-1} \binom{p-1}{n_{i-1} - 1} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_i} \right) \otimes \zeta^{\mathfrak{m}}\binom{\ldots, 1, \ldots}{\ldots, \varepsilon_{i-1}\varepsilon_i, \ldots} \\
&\quad + \delta_{n_r \leq p \leq n_r + n_{r-1} - 1} (-1)^{p-n_r} \binom{p-1}{p-n_r} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_r} \\
&\qquad \otimes \zeta^{\mathfrak{m}}\binom{\ldots, n_{r-1} + n_r - p}{\ldots, \varepsilon_{r-1}\varepsilon_r} \\
&\quad + \delta_{\substack{p = n_r + n_{r-1} - 1 \\ \varepsilon_{r-1}\varepsilon_r \neq 1}} (-1)^{n_r - 1} \left(\binom{p-1}{n_r - 1} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_{r-1}^{-1}} \right. \\
&\qquad \left. - \binom{p-1}{n_{r-1} - 1} \zeta^{\mathfrak{l}}\binom{p}{\varepsilon_r} \right) \otimes \zeta^{\mathfrak{m}}\binom{\ldots, 1}{\ldots, \varepsilon_{r-1}\varepsilon_r},
\end{aligned}$$

where δ is the function taking 1 exactly when the conditions on the subscript are satisfied, and taking 0 otherwise. The notion of $\zeta^{\mathfrak{m}}$ with "$\cdots$" in the image means that taking $\zeta^{\mathfrak{m}}\binom{n_1, \ldots, n_r}{\varepsilon_1, \ldots, \varepsilon_r}$ and replacing the $(i-1)$th or ith terms with a single term that is written. For example,

$$\zeta^{\mathfrak{m}}\binom{\ldots, n_i + n_{i-1} - p, \ldots}{\ldots, \varepsilon_{i-1}\varepsilon_i, \ldots} = \zeta^{\mathfrak{m}}\binom{n_1, \ldots, n_{i-2}, n_i + n_{i-1} - p, n_{i+1}, \ldots, n_r}{\varepsilon_1, \ldots, \varepsilon_{i-2}, \varepsilon_{i-1}\varepsilon_i, \varepsilon_{i+1} \ldots, \varepsilon_r}.$$

Remark. There is a typo in one sign in [15, Lemma 2.8].

For $N = 2, 3$, we have the following relations in depth 1 due to Deligne and Goncharov [11], where $\zeta^{\mathfrak{l}}$ denotes the image of $\zeta^{\mathfrak{m}}$ in $\mathcal{L}$.

- For $N = 2$,
$$(2^{-2n} - 1)\zeta^{\mathfrak{l}}\binom{2n+1}{1} = \zeta^{\mathfrak{l}}\binom{2n+1}{-1}. \tag{8.2.2}$$
- For $N = 3$,
$$\begin{aligned} \zeta^{\mathfrak{l}}\binom{2n+1}{1}(1 - 3^{2n}) = 2 \cdot 3^{2n}\zeta^{\mathfrak{l}}\binom{2n+1}{\varepsilon_3}, \quad \zeta^{\mathfrak{l}}\binom{2n}{1} = 0, \\ \zeta^{\mathfrak{l}}\binom{n}{\varepsilon_3} = (-1)^{n-1}\zeta^{\mathfrak{l}}\binom{n}{\varepsilon_3^{-1}}, \end{aligned} \tag{8.2.3}$$
  where $\varepsilon_3 = e^{\frac{2\pi\sqrt{-1}}{3}}$.

For $N = 2, 3$, by using the above relations in depth 1, Glanois [15, Definition 2.6] defined the following analogous derivations to those defined by Brown for $N = 1$.

Definition 8.2.2 (Glanois)**.** For each integer p and $\eta \in \mu_N$, define
$$\partial_p^\eta : \mathrm{gr}_r^{\mathfrak{D}}\mathcal{H}^N \to \mathrm{gr}_{r-1}^{\mathfrak{D}}\mathcal{H}^N, \tag{8.2.4}$$
as the composition of D_p followed by the projection:
$$\begin{aligned} \pi^\eta : \mathrm{gr}_1^{\mathfrak{D}}\mathcal{L}_p^N \otimes \mathrm{gr}_{r-1}^{\mathfrak{D}}\mathcal{H}^N &\to \mathrm{gr}_{r-1}^{\mathfrak{D}}\mathcal{H}^N \\ \zeta^{\mathfrak{l}}\binom{p}{\varepsilon} \otimes X &\mapsto c_{\eta,\varepsilon,p}X, \end{aligned}$$
with $c_{\eta,\varepsilon,p} \in \mathbb{Q}$ the coefficient of $\zeta^{\mathfrak{l}}\binom{p}{\eta}$ in the decomposition of $\zeta^{\mathfrak{l}}\binom{p}{\varepsilon}$ given by (8.2.2) or (8.2.3).

Let us fix the following basis of $\mathrm{gr}_1^{\mathfrak{D}}\mathcal{A}_p^N$:

- For $N=2$, take $\zeta^{\mathfrak{a}}\binom{p}{1}$ for odd $p \geq 1$.
- For $N=3$, take $\zeta^{\mathfrak{a}}\binom{p}{1}$ for odd $p \geq 1$, and $\zeta^{\mathfrak{a}}\binom{p}{\omega}$ for even $p \geq 2$.

Now for this basis, let us simplify our notation for ∂_p^{η} as follows:

- For $N=2$, write $\partial_p := \partial_p^1$ for odd $p \geq 1$.
- For $N=3$, write $\partial_p := \partial_p^1$ for odd $p \geq 1$, and $\partial_p := \partial_p^{\omega}$ for even $p \geq 2$.

Let $\mathbf{oo}(k)$ be the totally odd indexing set with the following order

$$\mathbf{oo}(k) = \{(k-3,3),(k-5,5),\cdots,(3,k-3)\},$$

and let us denote the reverse ordering indexing set to be $\mathbf{oo}'(k)$.

8.3 Two matrices and the explicit formulas

8.3.1 Definition of $\mathcal{C}_{k,2}^N$ and $\mathcal{D}_{k,2}^N$

Now we are ready to define the matrices $\mathcal{C}_{k,2}^N$ and $\mathcal{D}_{k,2}^N$.

Definition 8.3.1 (Definition of $\mathcal{C}_{k,2}^N$)**.** Let k be a positive even integer. For $N=2,3$, let $\varepsilon_N = e^{\frac{2\pi\sqrt{-1}}{N}}$. For any $(2m_1+1)+(2m_2+1)=(2n_1+1)+(2n_2+1)=k$, let us define

$$c^N_{\binom{2m_1+1\ 2m_2+1}{2n_1+1\ 2n_2+1}} = \partial_{2m_2+1}\partial_{2m_1+1}\zeta^{\mathfrak{m}}\begin{pmatrix}2n_1+1, 2n_2+1\\ \varepsilon_N, \varepsilon_N^{-1}\end{pmatrix} \in \mathbb{Q}. \tag{8.3.1}$$

We denote the matrix $\mathcal{C}_{k,2}^N$ as follows

$$\mathcal{C}_{k,2}^N = \left(c^N_{\binom{x}{y}}\right)_{\substack{x\in\mathbf{oo}(k)\\ y\in\mathbf{oo}'(k)}}. \tag{8.3.2}$$

Remark. Note that the $\mathcal{C}_{k,2}$ defined in Section 7.1.1 can also be defined as $\mathcal{C}^1_{k,2}$. Also note that we have ∂_1 when $N = 2, 3$, and ∂_{even} when $N = 3$, but here in the definition of $\mathcal{C}^N_{k,2}$ we still only consider ∂_p, with odd $p \geq 3$ as in the $\mathcal{C}^1_{k,2}$ case, since we want to set up connections with restricted even period polynomials.

Definition 8.3.2 (Definition of $\mathcal{D}^N_{k,2}$)**.** For any positive even integer k, and $N = 2, 3$, let us define $\mathcal{D}^N_{k,2}$ to be the diagonal matrix

$$\mathcal{D}^N_{k,2} = \left(\delta\binom{m_1, m_2}{n_1, n_2} \cdot c^{-1}_{1,\varepsilon_N,m_1}\right)_{\substack{(m_1,m_2)\in\mathbf{oo}(k)\\(n_1,n_2)\in\mathbf{oo}(k)}}, \tag{8.3.3}$$

where $\varepsilon_N = e^{\frac{2\pi\sqrt{-1}}{N}}$ and $c_{1,\varepsilon_N,p} \in \mathbb{Q}$ is the coefficient of $\zeta^{\mathfrak{l}}\binom{p}{1}$ in the decomposition of $\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N}$ given in (8.2.2) and (8.2.3), i.e.,

$$c_{1,1,p} = 1, \quad c_{1,-1,p} = (2^{-p+1} - 1), \quad c_{1,\varepsilon_3,p} = c_{1,\varepsilon_3^{-1},p} = \frac{3^{-p+1} - 1}{2}$$

for odd integers $p \geq 1$.

8.3.2 Explicit formulas for $\mathcal{C}^N_{k,2}$ and $\mathcal{D}^N_{k,2} \cdot \mathcal{C}^N_{k,2}$

In this section, we will prove explicit formulas for both $\mathcal{C}^N_{k,2}$ and $\mathcal{D}^N_{k,2} \cdot \mathcal{C}^N_{k,2}$.

Lemma 8.3.3. *Let $N = 2, 3$, let k be a positive even integer, and let $(m_1, m_2) \in \mathbf{oo}(k)$ and $(n_1, n_2) \in \mathbf{oo}'(k)$. We have*

$$(\mathcal{C}^N_{k,2})_{\binom{m_1,m_2}{n_1,n_2}} = c_{1,\varepsilon_N,m_1}\left(\delta\binom{m_1, m_2}{n_1, n_2} c_{1,\varepsilon_N,m_2} + (-1)^{n_1}\binom{m_1 - 1}{m_1 - n_1} + (-1)^{m_1-n_2}\binom{m_1 - 1}{m_1 - n_2}\right), \tag{8.3.4}$$

where $c_{1,\varepsilon_N,p} \in \mathbb{Q}$ is as in Definition 8.3.2.

Proof. For $N = 2, 3$, and odd $p \geq 3$, let us first compute D_p and ∂_p explicitly on the elements $\zeta^{\mathfrak{m}}\binom{n}{\varepsilon}$ for an Nth root of unity ε and $\zeta^{\mathfrak{m}}\binom{n_1, n_2}{\varepsilon_N, \varepsilon_N^{-1}}$ for $\varepsilon_N = e^{\frac{2\pi\sqrt{-1}}{N}}$ by using Proposition 8.2.1, (8.2.2), and (8.2.3).

When $r = 1$, we have

$$D_p : \zeta^{\mathfrak{m}}\binom{n}{\varepsilon} \longmapsto \delta_{p=n}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon}. \tag{8.3.5}$$

When $r = 2$, we have

$$\begin{aligned} D_p : \zeta^{\mathfrak{m}}\binom{n_1, n_2}{\varepsilon_N, \varepsilon_N^{-1}} \quad \mapsto \quad & \delta_{p=n_1}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N} \otimes \zeta^{\mathfrak{m}}\binom{n_2}{\varepsilon_N^{-1}} \\ & + \delta_{n_1 \leq p < n_1+n_2-1}(-1)^{n_1}\binom{p-1}{p-n_1}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N^{-1}} \\ & \qquad \otimes \zeta^{\mathfrak{m}}\binom{n_1+n_2-p}{1} \\ & + \delta_{n_2 \leq p \leq n_1+n_2-1}(-1)^{p-n_2}\binom{p-1}{p-n_2}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N^{-1}} \\ & \qquad \otimes \zeta^{\mathfrak{m}}\binom{n_1+n_2-p}{1}. \end{aligned} \tag{8.3.6}$$

If we use the convention that $\binom{r}{s} = 0$ if $s < 0 < r$ and $\zeta^{\mathfrak{m}}\binom{n}{1} = 0$ if $n \leq 0$, the above expression can be simplified to

$$\begin{aligned} D_p : \zeta^{\mathfrak{m}}\binom{n_1, n_2}{\varepsilon_N, \varepsilon_N^{-1}} \quad \mapsto \quad & \delta_{p=n_1}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N} \otimes \zeta^{\mathfrak{m}}\binom{n_2}{\varepsilon_N^{-1}} \\ & + (-1)^{n_1}\binom{p-1}{p-n_1}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N^{-1}} \otimes \zeta^{\mathfrak{m}}\binom{n_1+n_2-p}{1} \\ & + (-1)^{p-n_2}\binom{p-1}{p-n_2}\zeta^{\mathfrak{l}}\binom{p}{\varepsilon_N^{-1}} \otimes \zeta^{\mathfrak{m}}\binom{n_1+n_2-p}{1}. \end{aligned} \tag{8.3.7}$$

Now from (8.3.5) and (8.3.7), when $(m_1, m_2) \in \mathbf{oo}(k)$ and $(n_1, n_2) \in \mathbf{oo}'(k)$, we have

$$\begin{aligned} & (\mathcal{C}_{k,2}^N)_{\binom{m_1, m_2}{n_1, n_2}} \\ = \quad & \partial_{m_2}\partial_{m_1}\zeta^{\mathfrak{m}}\binom{n_1, n_2}{\epsilon_N, \epsilon_N^{-1}} \end{aligned}$$

$$
\begin{aligned}
&= c_{1,\varepsilon_N,m_1}\partial_{m_2}\Bigg(\delta_{m_1=n_1}\zeta^{\mathfrak{m}}\binom{n_2}{\varepsilon_N^{-1}} + (-1)^{n_1}\binom{m_1-1}{m_1-n_1}\zeta^{\mathfrak{m}}\binom{n_1+n_2-m_1}{1} \\
&\qquad\qquad + (-1)^{m_1-n_2}\binom{m_1-1}{m_1-n_2}\zeta^{\mathfrak{m}}\binom{n_1+n_2-m_1}{1}\Bigg) \\
&= c_{1,\varepsilon_N,m_1}\left(\delta\binom{m_1,m_2}{n_1,n_2}c_{1,\varepsilon_N,m_2} + (-1)^{n_1}\binom{m_1-1}{m_1-n_1} + (-1)^{m_1-n_2}\binom{m_1-1}{m_1-n_2}\right).
\end{aligned}
$$

□

From the above lemma and (8.3.3), we have the following explicit formula for $\mathcal{D}^N_{k,2}\cdot\mathcal{C}^N_{k,2}$

Lemma 8.3.4. *Let $N=2,3$, and let k be a positive even integer. We have*

$$
(\mathcal{D}^N_{k,2}\cdot\mathcal{C}^N_{k,2})_{\binom{m_1,m_2}{n_1,n_2}} = \delta\binom{m_1,m_2}{n_1,n_2}c_{1,\varepsilon_N,m_2} + (-1)^{n_1}\binom{m_1-1}{m_1-n_1} + (-1)^{m_1-n_2}\binom{m_1-1}{m_1-n_2}, \tag{8.3.8}
$$

where (m_1,m_2) runs over $\mathbf{oo}(k)$ and (n_1,n_2) runs over $\mathbf{oo}'(k)$.

8.4 Two theorems

As described in Section 4.4.1, Baumard and Schneps' result can be reformulated as the following theorem.

Theorem 8.4.1 (Reformulation of Proposition 4.4.1)**.** *Let k be an even integer. The left kernel of $\mathcal{C}^1_{k,2}$ consisits exactly of those vectors coming from the restricted even period polynomials of cusp forms of weight k for $\mathrm{SL}_2(\mathbb{Z})$.*

Now we can generalize this result to the case that $N=2,3$.

Theorem 8.4.2 (Connection with Hecke operators)**.** *Let k be an even integer. When $N=2,3$, the vectors coming from the restricted even period polynomials of cuspidal* *eigenforms of weight k for $\mathrm{SL}_2(\mathbb{Z})$ are left eigenvectors of $\mathcal{C}_{k,2}^N$, and the corresponding eigenvalues are given by*

- $N = 2$,
$$\frac{\lambda_2 - (1 + 2^{k-1})}{2^{k-2}}, \tag{8.4.1}$$

- $N = 3$,
$$\frac{\lambda_3 - (1 + 3^{k-1})}{4 \cdot 3^{k-2}}, \tag{8.4.2}$$

where λ_2 (respectively, λ_3) is the eigenvalue of the Hecke operator T_2 (respectively, T_3) for the corresponding eigenform.

We will also prove the following result for the product $\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N$.

Theorem 8.4.3 (Connection with newforms)**.** *Let k be an even integer. When $N = 2, 3$, the vectors coming from the restricted even period polynomials of newforms of weight k and level $\Gamma_1(N)$ are left eigenvectors of $(\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N)$, and the corresponding eigenvalues are given by*

- $N = 2$,
$$-\left(1 + \frac{\varepsilon}{2^{\frac{k-2}{2}}}\right), \tag{8.4.3}$$

- $N = 3$,
$$-\frac{1}{2}\left(1 + \frac{\varepsilon}{3^{\frac{k-2}{2}}}\right), \tag{8.4.4}$$

where $\varepsilon \in \{\pm 1\}$ is the eigenvalue of the Atkin-Lehner involution W_N on the corresponding newform.

Remark. It is worth mentioning that in the proofs of Theorems 8.4.2 (see (8.5.7) and (8.5.8)) and 8.4.3 (see (8.6.4) and (8.6.5)), we can see that the actions of $\mathcal{C}_{k,2}^N$ and $\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N$ are nothing but the following two well-known operators (up to scalar) on the corresponding spaces:

$$\mathcal{C}_{k,2}^N \quad \longleftrightarrow \quad T_N - 1 - N^{k-1} \text{ acting on } r_f^{-,0}(x,y) \text{ of } f \in \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z})), \tag{8.4.5}$$

$$\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N \quad \longleftrightarrow \quad U_N - 1 \qquad \text{acting on } r_f^{-,0}(x,y) \text{ of } f \in \mathcal{S}_k^{\mathrm{new}}(\Gamma_1(N))^{\pm}, \tag{8.4.6}$$

where $r_f^{-,0}(x,y)$ is the restricted even period polynomial of f. We can see that Theorems 8.4.2 and 8.4.3 are compatible with Proposition 4.4.1, since when $N=1$ both $\mathcal{C}_{k,2}^N$ and $\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N$ give us the $T_1 - 1 = U_1 - 1 = 0$ action on the restricted even period polynomials of $f \in \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ (in this case, $\mathcal{S}_k^{\mathrm{new}}(\mathrm{SL}_2(\mathbb{Z})) = \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$).

8.5 Proof of Theorem 8.4.2

In this section, we will give the proof of Theorem 8.4.2. First, we want to introduce the representative sets of the Hecke operators T_2, T_3 acting on the period polynomial spaces. The following result is due to Zagier [37, Theorem 2]. First recall Theorem 2.3.8 for T_2 and T_3.

Theorem 8.5.1 (Zagier)**.** *The representative sets of the Hecke operators T_2, T_3 acting on the even period polynomial spaces are given by*

$$\boldsymbol{Man_2} = \left\{ \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix} \right\},$$

$$\boldsymbol{Man_3} = \left\{ \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}, \begin{pmatrix} 3 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 3 & 0 \\ -1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 3 \end{pmatrix}, \begin{pmatrix} 1 & -1 \\ 0 & 3 \end{pmatrix} \right\}.$$

Now we are ready to prove Theorem 8.4.2.

Proof of Theorem 8.4.2. When $N = 2$, for any $(m_1, m_2) \in \mathbf{oo}(k)$ and $(n_1, n_2) \in \mathbf{oo}'(k)$, let us set

$$e\binom{m_1, m_2}{n_1, n_2} = (-1)^{n_1}\binom{m_1 - 1}{m_1 - n_1} + (-1)^{m_1 - n_2}\binom{m_1 - 1}{m_1 - n_2}.$$

This e is exactly the main term in the definition of $(\mathcal{C}^1_{k,2})_{\binom{m_1,m_2}{n_1,n_2}}$, i.e.,

$$(\mathcal{C}^1_{k,2})_{\binom{m_1,m_2}{n_1,n_2}} = \delta\binom{m_1, m_2}{n_1, n_2} + e\binom{m_1, m_2}{n_1, n_2}.$$

From Lemma 8.3.3, we have

$$\begin{aligned}
(\mathcal{C}^2_{k,2})_{\binom{m_1,m_2}{n_1,n_2}} &= c_{1,-1,m_1}\left(\delta\binom{m_1, m_2}{n_1, n_2}c_{1,-1,m_2} + e\binom{m_1, m_2}{n_1, n_2}\right) \\
&= (2^{-m_1+1} - 1)(2^{-m_2+1} - 1)\delta\binom{m_1, m_2}{n_1, n_2} + (2^{-m_1+1} - 1)e\binom{m_1, m_2}{n_1, n_2} \\
&= -2^{-m_1+1}\delta\binom{m_1, m_2}{n_1, n_2} - 2^{-m_2+1}\delta\binom{m_1, m_2}{n_1, n_2} + 2^{-m_1+1}e\binom{m_1, m_2}{n_1, n_2} \\
&\quad -(\mathcal{C}^1_{k,2})_{\binom{m_1,m_2}{n_1,n_2}} + 2\delta\binom{m_1, m_2}{n_1, n_2} + 2^{-k+2}\delta\binom{m_1, m_2}{n_1, n_2}
\end{aligned}$$

Define

$$\begin{aligned}
A_{\binom{m_1,m_2}{n_1,n_2}} &:= 2^{-m_1+1}\delta\binom{m_1, m_2}{n_1, n_2}, \\
B_{\binom{m_1,m_2}{n_1,n_2}} &:= 2^{-m_2+1}\delta\binom{m_1, m_2}{n_1, n_2}, \\
C_{\binom{m_1,m_2}{n_1,n_2}} &:= 2^{-m_1+1}e\binom{m_1, m_2}{n_1, n_2}.
\end{aligned}$$

Then we have the following decomposition

$$\mathcal{C}^2_{k,2} = -A - B + C - \mathcal{C}^1_{k,2} + 2J + 2^{-k+2}J, \tag{8.5.1}$$

where J is the exchange matrix, i.e., the anti-diagonal matrix with all nonzero entries equal to 1. For any eigenform f of weight k and level $\mathrm{SL}_2(\mathbb{Z})$, let $r_f(x, y)$ be its period polynomial

$$r_f(x,y) = \int_0^{i\infty} f(z)(zy-x)^{k-2}dz.$$

The restricted even part of this period polynomial is

$$r_f^{-,0}(x,y) = \sum_{(m_1,m_2)\in\mathbf{oo}(k)} a_{m_1,m_2} x^{m_2-1} y^{m_1-1}.$$

We associate to this restricted even period polynomial the following vector

$$v = (a_{m_1,m_2})_{(m_1,m_2)\in\mathbf{oo}(k)}. \tag{8.5.2}$$

By the definition of the matrices A, B, C, J, we have the following maps $\mathbb{Q}[x, y] \to \mathbb{Q}[x, y]$:

$$\cdot A \quad : \quad p(x,y) \mapsto p(\frac{y}{2}, x), \tag{8.5.3}$$

$$\cdot B \quad : \quad p(x,y) \mapsto p(y, \frac{x}{2}), \tag{8.5.4}$$

$$\cdot C \quad : \quad p(x,y) \mapsto p(x, \frac{x+y}{2}) - p(y, \frac{x+y}{2}), \tag{8.5.5}$$

$$\cdot J \quad : \quad p(x,y) \mapsto p(y,x). \tag{8.5.6}$$

By Theorem 8.4.1, we also know that

$$\cdot\mathcal{C}_{k,2}^1 : r_f^{-,0}(x,y) \mapsto 0.$$

Therefore, we have

$$\cdot\mathcal{C}_{k,2}^2 : r_f^{-,0}(x,y) \quad \mapsto \quad -r_f^{-,0}(\frac{y}{2}, x) - r_f^{-,0}(y, \frac{x}{2}) + r_f^{-,0}(x, \frac{x+y}{2}) - r_f^{-,0}(y, \frac{x+y}{2})$$

$$\begin{aligned}
&+(2+2^{-k+2})r_f^{-,0}(y,x)\\
=\ & r_f^{-,0}(x,\frac{y}{2})+r_f^{-,0}(\frac{x}{2},y)+r_f^{-,0}(x,\frac{x+y}{2})+r_f^{-,0}(\frac{x+y}{2},y)\\
&-(2+2^{-k+2})r_f^{-,0}(x,y)\\
=\ & 2^{-k+2}\Big(r_f^{-,0}(2x,y)+r_f^{-,0}(x,2y)+r_f^{-,0}(2x,x+y)\\
&+r_f^{-,0}(x+y,2y)\Big)-(2+2^{-k+2})r_f^{-,0}(x,y)
\end{aligned}$$

From Theorem 8.5.1, if f is an eigenform with T_2-eigenvalue λ_2, we have

$$r_f^{-,0}(2x,y)+r_f^{-,0}(x,2y)+r_f^{-,0}(2x,x+y)+r_f^{-,0}(x+y,2y)=r_{T_2f}^{-,0}(x,y)=\lambda_2 r_f^{-,0}(x,y).$$

Therefore,

$$\begin{aligned}
\cdot\mathcal{C}_{k,2}^2: r_f^{-,0}(x,y)\ &\mapsto\ (2^{-k+2}\lambda_2-2-2^{-k+2})r_f^{-,0}(x,y) \qquad (8.5.7)\\
&=\ \frac{\lambda_2-(1+2^{k-2})}{2^{k-2}}r_f^{-,0}(x,y).
\end{aligned}$$

Hence we have proven the statement for $N=2$.

Now let us prove it for $N=3$. By the analogous computation, we have

$$\begin{aligned}
\cdot\mathcal{C}_{k,2}^3: r_f^{-,0}(x,y)\ &\mapsto\ \frac{1}{4}r_f^{-,0}(x,\frac{y}{3})+\frac{1}{4}r_f^{-,0}(\frac{x}{3},y)+\frac{1}{2}r_f^{-,0}(x,\frac{x+y}{3})+\frac{1}{2}r_f^{-,0}(\frac{x+y}{3},y)\\
&\quad -\frac{1}{4}(3+3^{-k+2})r_f^{-,0}(x,y)\\
&=\ \frac{3^{-k+2}}{4}\Big(r_f^{-,0}(3x,y)+r_f^{-,0}(x,3y)+2r_f^{-,0}(3x,x+y)\\
&\quad +2r_f^{-,0}(x+y,3y)\Big)-\frac{3+3^{-k+2}}{4}r_f^{-,0}(x,y),
\end{aligned}$$

where $\frac{1}{2}$ and $\frac{1}{4}$ are coming from the $\frac{1}{2}$ in the identity

$$c_{1,\varepsilon_3,p}=c_{1,\varepsilon_3^{-1},p}=\frac{3^{-p+1}-1}{2}.$$

Now since $r_f^{-,0}(x,y)$ is an even polynomial, and we only need the even degree part in the final expression, we have

$$\begin{aligned} 2r_f^{-,0}(3x,x+y) &\equiv r_f^{-,0}(3x,x+y)+r_f^{-,0}(3x,x-y) \qquad \pmod{x^{\text{odd}}y^{\text{odd}}}, \\ 2r_f^{-,0}(x+y,xy) &\equiv r_f^{-,0}(x+y,3y)+r_f^{-,0}(x-y,3y) \qquad \pmod{x^{\text{odd}}y^{\text{odd}}}. \end{aligned}$$

Therefore, we have

$$\begin{aligned} \cdot\mathcal{C}_{k,2}^3 : p(x,y) &\mapsto \frac{3^{-k+2}}{4}\Big(r_f^{-,0}(3x,y)+r_f^{-,0}(x,3y)+2r_f^{-,0}(3x,x+y) \\ &\quad +2r_f^{-,0}(x+y,3y)\Big)-\frac{3+3^{-k+2}}{4}r_f^{-,0}(x,y) \\ &= \frac{3^{-k+2}}{4}r_{T_3f}^{-,0}(x,y)-\frac{3+3^{-k+2}}{4}r_f^{-,0}(x,y) \\ &= \frac{\lambda_3-(1+3^{k-1})}{4\cdot 3^{k-2}}r_f^{-,0}(x,y). \end{aligned} \tag{8.5.8}$$

Hence we have also proven the statement for $N=3$. □

8.6 Proof of Theorem 8.4.3

8.6.1 Actions of U_2 and U_3 on period polynomials

In this section, we will prove a result about the U_N-operator acting on period polynomials of cusp form of weight k and level $\Gamma_1(N)$ for $N=2,3$.

Lemma 8.6.1. *Fix $f\in\mathcal{S}_k(\Gamma_1(2))$, and let $r_f(x,y)$ denote its period polynomial. Then we have*

$$r_{U_2f}(x,y)=r_f(x,2y)+r_f(x+y,2y)-r_f(x+y,-2x). \tag{8.6.1}$$

Proof. For $f \in \mathcal{S}_k(\Gamma_1(2))$, the matrices $\left(\begin{smallmatrix}1&0\\0&2\end{smallmatrix}\right)$ and $\left(\begin{smallmatrix}1&1\\0&2\end{smallmatrix}\right)$ form a system of coset representatives for the U_2-operator. Then we have

$$\begin{aligned}
r_{U_2f}(x,y) &= \int_0^{i\infty} \frac{1}{2} f\left(\frac{z}{2}\right)(zy-x)^{k-2}dz + \int_0^{i\infty} \frac{1}{2} f\left(\frac{z+1}{2}\right)(zy-x)^{k-2}dz \\
&= \int_0^{i\infty} f(z)(2zy-x)^{k-2}dz + \int_{\frac{1}{2}}^{i\infty} f(z)((2z-1)y-x)^{k-2}dz \\
&= \int_0^{i\infty} f(z)(2yz-x)^{k-2}dz + \left(\int_0^{i\infty} - \int_0^{\frac{1}{2}}\right) f(z)(2yz-(x+y))^{k-2}dz \\
&= r_f(x,2y) + r_f(x+y,2y) - \int_0^{\frac{1}{2}} f(z)(2yz-(x+y))^{k-2}dz \\
&= r_f(x,2y) + r_f(x+y,2y) - \int_0^{i\infty} f(\gamma z)(2y\gamma(z)-(x+y))^{k-2}d\gamma(z), \\
&= r_f(x,2y) + r_f(x+y,2y) \\
&\quad - \int_0^{i\infty} (2z+1)^k (f|_k\gamma)(z)\frac{1}{(2z+1)^k}(-2xz-(x+y))^{k-2}dz \\
&= r_f(x,2y) + r_f(x+y,2y) - \int_0^{i\infty} f(z)(-2xz-(x+y))^{k-2}dz \\
&= r_f(x,2y) + r_f(x+y,2y) - r_f(x+y,-2x),
\end{aligned}$$

where $\gamma = \left(\begin{smallmatrix}1&0\\2&1\end{smallmatrix}\right) \in \Gamma_1(2)$. $\square$

Lemma 8.6.2. *For any $f \in \mathcal{S}_k(\Gamma_1(3))$, let $r_f(x,y)$ denote its period polynomial, then we have*

$$r_{U_3f}(x,y) = r_f(x,3y)+r_f(x+y,3y)-r_f(x+y,-3x)+r_f(x-y,3y)-r_f(-(x-y),-3x) \tag{8.6.2}$$

Proof. For $f \in \mathcal{S}_k(\Gamma_1(3))$, the matrices $\left(\begin{smallmatrix}1&0\\0&3\end{smallmatrix}\right)$, $\left(\begin{smallmatrix}1&1\\0&3\end{smallmatrix}\right)$, and $\left(\begin{smallmatrix}1&2\\0&3\end{smallmatrix}\right)$ form a system of coset representatives for the U_3-operator. Then we have

$$r_{U_3f}(x,y)$$

$$
\begin{aligned}
&= \sum_{j=0}^{2}\int_0^{i\infty}\frac{1}{3}f\left(\frac{z+j}{3}\right)(zy-x)^{k-2}dz \\
&= \sum_{j=0}^{2}\int_{\frac{j}{3}}^{i\infty} f(z)((3z-j)y-x)^{k-2}dz \\
&= \int_0^{i\infty} f(z)(3yz-x)^{k-2}dz + \left(\int_0^{i\infty} - \int_0^{\frac{1}{3}}\right) f(z)(3yz-(x+y))^{k-2}dz \\
&\qquad + \left(\int_1^{i\infty} - \int_1^{\frac{2}{3}}\right) f(z)(3yz-(x+2y))^{k-2}dz \\
&= r_f(x,3y) + r_f(x+y,3y) - \int_0^{\frac{1}{3}} f(z)(3yz-(x+y))^{k-2}dz \\
&\qquad + \int_1^{i\infty} f(z)(3yz-(x+2y))^{k-2}dz - \int_1^{\frac{2}{3}} f(z)(3yz-(x+2y))^{k-2}dz.
\end{aligned}
$$

Now let us compute the last three integrals:

$$
\begin{aligned}
\int_0^{\frac{1}{3}} f(z)(3yz-(x+y))^{k-2}dz &= \int_0^{i\infty} f(\gamma_1 z)(3y\gamma_1(z)-(x+y))^{k-2}d\gamma_1(z) \\
&= \int_0^{i\infty} f(z)(-3xz-(x+y))^{k-2}dz \\
&= r_f(x+y,-3x),
\end{aligned}
$$

where $\gamma_1 = \left(\begin{smallmatrix} 1 & 0 \\ 3 & 1 \end{smallmatrix}\right) \in \Gamma_1(3)$.

$$
\begin{aligned}
\int_1^{i\infty} f(z)(3yz-(x+2y))^{k-2}dz &= \int_0^{i\infty} f(\gamma_2 z)(3y\gamma_2(z)-(x+2y))^{k-2}d\gamma_2(z), \\
&= \int_0^{i\infty} f(z)(3yz-(x-y))^{k-2}dz \\
&= r_f(x-y,3y),
\end{aligned}
$$

where $\gamma_2 = \left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right) \in \Gamma_1(3)$.

$$
\int_1^{\frac{2}{3}} f(z)(3yz-(x+2y))^{k-2}dz = \int_0^{i\infty} f(\gamma_3 z)(3y\gamma_3(z)-(x+2y))^{k-2}d\gamma_3(z),
$$

$$
\begin{aligned}
&= \int_0^{i\infty} f(z)(-3xz + (x-y))^{k-2}dz \\
&= r_f(-(x-y), -3x),
\end{aligned}
$$

where $\gamma_3 = \left(\begin{smallmatrix} -2 & 1 \\ -3 & 1 \end{smallmatrix}\right) \in \Gamma_1(3)$. Therefore, we have the desired formula. □

In particular, (8.6.1) and (8.6.2) also hold for restricted even period polynomials. We also need the following fact about the action of the Atkin-Lehner involution W_N on $\mathcal{S}_k(\Gamma_1(N))$ of Definition 2.3.7. Recall from (2.3.1) that we can decompose $\mathcal{S}_k(\Gamma_1(N))$ into two eigenspaces $\mathcal{S}_k(\Gamma_1(N))^{\pm}$ such that

$$\mathcal{S}_k(\Gamma_1(N))^{\pm} = \{f \in \mathcal{S}_k(\Gamma_1(N)) \mid W_N f = \pm f\}.$$

For each $f \in \mathcal{S}_k(\Gamma_1(N))^{\pm}$, denote its Atkin-Lehner eigenvalue by ε_f. For the corresponding period polynomial, we then have

$$
\begin{aligned}
N^{\frac{k-2}{2}}\varepsilon_f \cdot r_f(x,y) &= r_{f|_k\left(\begin{smallmatrix} 0 & -1 \\ N & 0 \end{smallmatrix}\right)}(x,y) \\
&= \int_0^{i\infty} N^{k-1}\frac{1}{(Nz)^k} f(\frac{-1}{Nz})(zy-x)^{k-2}dz \\
&= \int_{i\infty}^{0} N^{k-1}(-z)^k f(z)\left(\frac{-y}{Nz} - x\right)^{k-2} d\left(\frac{-1}{Nz}\right) \\
&= -\int_0^{i\infty} f(z)(xNz+y)^{k-2}dz \\
&= -r_f(-y, Nx).
\end{aligned}
$$

Therefore, for the restricted even period polynomial of $f \in \mathcal{S}_k(\Gamma_1(N))^{\pm}$, we have

$$r_f^{-,0}(y, Nx) = -N^{\frac{k-2}{2}}\varepsilon_f \cdot r_f^{-,0}(x,y) \tag{8.6.3}$$

8.6.2 Proof of Theorem 8.4.3

Now we are ready to prove Theorem 8.4.3.

Proof of Theorem 8.4.3. When $N = 2$, as in the proof of Theorem 8.4.2, we know that for any $f \in \mathcal{S}_k^{\text{new}}(\Gamma_1(2))^{\pm}$, by Lemma 8.6.1, we have

$$\begin{aligned}
\cdot(\mathcal{D}_{k,2}^2 \cdot \mathcal{C}_{k,2}^2) : r_f^{-,0}(x,y) &\mapsto -r_f^{-,0}(y,x) - r_f^{-,0}(y,x+y) + r_f^{-,0}(x,x+y) + r_f^{-,0}\left(\frac{y}{2}, x\right) \\
&= \frac{\varepsilon_f}{2^{\frac{k-2}{2}}}\Big(r_f^{-,0}(x,2y) + r_f^{-,0}(x+y,2y) - r_f^{-,0}(x+y,2x) \\
&\qquad -r_f^{-,0}(x,y)\Big) \\
&= \frac{\varepsilon_f}{2^{\frac{k-2}{2}}} \cdot \Big(r_{U_2 f}^{-,0}(x,y) - r_f^{-,0}(x,y)\Big) \qquad (8.6.4)
\end{aligned}$$

where the first two lines are considered modulo $(x^{k-2} - y^{k-2})$. Note that in the first line, we already know that the expression only contains even degree terms, so we do not need to cancel the odd degree terms. Now since

$$\begin{aligned}
&\frac{\varepsilon_f}{2^{\frac{k-2}{2}}} \cdot \Big(r_{U_2 f}^{-,0}(x,y) - r_f^{-,0}(x,y)\Big) \\
= \; &\frac{\varepsilon_f}{2^{\frac{k-2}{2}}} \cdot \Big(-2^{\frac{k-2}{2}}\varepsilon_f \cdot r_f^{-,0}(x,y) - r_f^{-,0}(x,y)\Big) \\
= \; &\left(-1 - \frac{\varepsilon_f}{2^{\frac{k-2}{2}}}\right) r_f^{-,0}(x,y),
\end{aligned}$$

we have shown the statement for $N = 2$.

When $N = 3$, for any restricted even period polynomial $r_f^{-,0}(X,Y)$ of $f \in \mathcal{S}_k^{\text{new}}(\Gamma_1(3))^{\pm}$, we have

$$\cdot(\mathcal{D}_{k,2}^3 \cdot \mathcal{C}_{k,2}^3) : r_f^{-,0}(x,y) \mapsto \frac{1}{2}\Big(-\frac{1}{2} r_f^{-,0}(y,x) - r_f^{-,0}(y,x+y) + r_f^{-,0}(x,x+y)\Big)$$

$$
\begin{aligned}
& +\frac{1}{2}\Big(-\frac{1}{2} r_f^{-,0}(-y,x) - r_f^{-,0}(-y,x-y) + r_f^{-,0}(x,x-y)\Big) \\
& +\frac{1}{2} r_f^{-,0}\Big(\frac{y}{3},x\Big) \\
= \;& \frac{1}{2}\Big(- r_f^{-,0}(y,x) - r_f^{-,0}(y,x+y) + r_f^{-,0}(x,x+y) \\
& - r_f^{-,0}(y,x-y) + r_f^{-,0}(x,x-y)\Big) + \frac{1}{2} r_f^{-,0}\Big(\frac{y}{3},x\Big) \\
= \;& \frac{\varepsilon_f}{2\cdot 3^{\frac{k-2}{2}}}\Big(r_f^{-,0}(x,3y) + r_f^{-,0}(x+y,3y) - r_f^{-,0}(x+y,3x) \\
& \qquad + r_f^{-,0}(x-y,3y) - r_f^{-,0}(x-y,3x) - r_f^{-,0}(x,y)\Big) \\
= \;& \frac{\varepsilon_f}{2\cdot 3^{\frac{k-2}{2}}}\cdot\Big(r_{U_3 f}^{-,0}(x,y) - r_f^{-,0}(x,y)\Big) \qquad (8.6.5)
\end{aligned}
$$

where the first two lines are considered modulo $(x^{k-2}-y^{k-2})$. We split the first term in the first line here into two parts since we want to cancel the odd degree terms. Now since

$$
\begin{aligned}
& \frac{\varepsilon_f}{2\cdot 3^{\frac{k-2}{2}}}\cdot\Big(r_{U_3 f}^{-,0}(x,y) - r_f^{-,0}(x,y)\Big) \\
= \;& \frac{\varepsilon_f}{2\cdot 3^{\frac{k-2}{2}}}\cdot\Big(- 3^{\frac{k-2}{2}}\varepsilon_f \cdot r_f^{-,0}(x,y) - r_f^{-,0}(x,y)\Big) \\
= \;& \Big(-\frac{1}{2} - \frac{\varepsilon_f}{2\cdot 3^{\frac{k-2}{2}}}\Big) r_f^{-,0}(x,y),
\end{aligned}
$$

we have also shown the statement for $N = 3$. □

8.7 Examples

In this section, we will provide some examples for Theorems 8.4.2 and 8.4.3.

Example 8.7.1. When $k = 12$, we have

$$\mathcal{C}^2_{12,2} = \begin{pmatrix} \frac{6885}{256} & \frac{5355}{128} & -\frac{5355}{128} & -\frac{26775}{1024} \\ \frac{945}{64} & \frac{441}{32} & -\frac{13167}{1024} & -\frac{945}{64} \\ \frac{45}{8} & \frac{1905}{1024} & -\frac{15}{16} & -\frac{45}{8} \\ \frac{1533}{1024} & 0 & 0 & -\frac{3}{4} \end{pmatrix}$$

$$\mathcal{C}^3_{12,2} = \begin{pmatrix} \frac{3280}{243} & \frac{45920}{2187} & -\frac{45920}{2187} & -\frac{783920}{59049} \\ \frac{1820}{243} & \frac{5096}{729} & -\frac{398216}{59049} & -\frac{1820}{243} \\ \frac{80}{27} & \frac{43720}{59049} & -\frac{40}{81} & -\frac{80}{27} \\ \frac{39364}{59049} & 0 & 0 & -\frac{4}{9} \end{pmatrix}$$

These two matrices both have one left eigenvector $(1, -3, 3, -1)$, and it corresponds to the restricted even period polynomial

$$r_f^{-,0}(x, y) = x^2y^8 - 3x^4y^6 + 3x^6y^4 - x^8y^2$$

of the unique cusp form in $\mathcal{S}_{12}(\mathrm{SL}_2(\mathbb{Z}))$. The corresponding eigenvalues are

- $N = 2$,
$$\frac{\lambda_2 - (1 + 2^{k-1})}{2^{k-2}} = -\frac{2073}{1024} = 691 \cdot \frac{-3}{1024},$$
- $N = 3$,
$$\frac{\lambda_3 - (1 + 3^{k-1})}{4 \cdot 3^{k-2}} = -\frac{44224}{59049} = 691 \cdot \frac{-64}{59049}.$$

Notice that the irregular prime 691 divides the numerator of the Bernoulli number B_{12}.

Remark. The divisibility of the irregular primes by B_k in the products of eigenvalues

$$\prod_{i=1}^{\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))} \frac{\lambda_{2,i} - (1 + 2^{k-1})}{2^{k-2}} \text{ and } \prod_{i=1}^{\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))} \frac{\lambda_{3,i} - (1 + 3^{k-1})}{4 \cdot 3^{k-2}}$$

arises from the well-known result [32, Proposition 3.5] on the congruences between Eisenstein series and cusp forms.

Example 8.7.2. When $k = 10$, we have

$$\mathcal{D}_{10,2}^{2} \cdot \mathcal{C}_{10,2}^{2} = \begin{pmatrix} -14 & 0 & \frac{53}{4} \\ -6 & -\frac{15}{16} & 6 \\ -\frac{127}{64} & 0 & 1 \end{pmatrix}$$

$$\mathcal{D}_{10,2}^{3} \cdot \mathcal{C}_{10,2}^{3} = \begin{pmatrix} -14 & 0 & \frac{122}{9} \\ -6 & -\frac{40}{81} & 6 \\ -\frac{1093}{729} & 0 & 1 \end{pmatrix}$$

The first matrix has one left eigenvector $(2, -7, 8)$ with eigenvalue $-\frac{15}{16}$, and this eigenvector corresponds to the restricted even period polynomial

$$r_f^{-,0}(x, y) = 2x^2y^6 - 7x^4y^4 + 8x^6y^2$$

of the unique newform in $\mathcal{S}_{10}^{\text{new}}(\Gamma_1(2))^-$. The second matrix has one left eigenvector $(2, -9, 18)$ with eigenvalue $-\frac{40}{81}$, and this eigenvector corresponds to the restricted even period polynomial

$$r_f^{-,0}(x, y) = 2x^2y^6 - 9x^4y^4 + 18x^6y^2$$

of the unique newform in $\mathcal{S}_{10}^{\text{new}}(\Gamma_1(3))^-$. It also has another left eigenvector $(1, 0, -9)$ with eigenvalue $-\frac{41}{81}$, and this eigenvector corresponds to the restricted even period polynomial

$$r_f^{-,0}(x, y) = x^2y^6 - 9x^6y^2$$

of the unique newform in $\mathcal{S}_{10}^{\text{new}}(\Gamma_1(3))^+$.

8.8 Applications

In this section, we will provide applications of Theorems 8.4.2 and 8.4.3. From Theorem 8.4.2, we know that when $N = 2, 3$, each eigenform $f \in \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ gives us a left eigenvector of $\mathcal{C}_{k,2}^N$ with eigenvalues

- $N = 2$,
$$\frac{\lambda_2 - (1 + 2^{k-1})}{2^{k-2}},$$
- $N = 3$,
$$\frac{\lambda_3 - (1 + 3^{k-1})}{4 \cdot 3^{k-2}}.$$

We have the following result due to Deligne [9], which gives an estimation of the coefficients of cusp forms.

Theorem 8.8.1 (Deligne)**.** *For any $f = \sum_{n=1}^{\infty} a_n q^n \in \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ and prime p, we have*
$$|a_p| \leq 2p^{\frac{k-1}{2}}.$$

Therefore, we can see the corresponding eigenvalues for eigenforms have the following asymptotical behavior:

$$\begin{aligned} \frac{\lambda_2 - (1 + 2^{k-1})}{2^{k-2}} &\to -2 \quad \text{as } k \to \infty, \\ \frac{\lambda_3 - (1 + 3^{k-1})}{4 \cdot 3^{k-2}} &\to -\frac{3}{4} \quad \text{as } k \to \infty. \end{aligned}$$

By a numerical computation up to weight ≤ 100, we found that the number of the eigenvalues close to -2 and $-\frac{3}{4}$ (close in the sense of the bound by Deligne) is exactly the dimension of space of cusp forms, which suggests that we can use $\mathcal{C}^2_{k,2}$ and $\mathcal{C}^3_{k,2}$ to compute the eigenvalues of the T_2 and T_3 operators and also to compute the period polynomials of eigenforms. One advantage of using these two matrices is that we have explicit formulas for them which only contain binomial coefficients.

From Theorem 8.4.3, we know that when $N = 2, 3$, each $f \in \mathcal{S}^{\text{new}}_k(\Gamma_1(N))^{\pm}$ gives us a left eigenvector of $(\mathcal{D}^N_{k,2} \cdot \mathcal{C}^N_{k,2})$ with eigenvalues described by the theorem. By a numerical computation up to weight ≤ 100, we found that the dimensions of eigenspaces match with the dimensions of the corresponding newform spaces, and hence we made the following conjecture. The summation starts from $k = 6$, since we already know that $\mathcal{S}^{\text{new}}_{<6}(\Gamma_1(N)) = 0$ when $N = 2, 3$, and also our method only works for $k \geq 6$ since $\mathbf{oo}(k) \neq \varnothing$ when $k \geq 6$.

Conjecture 8.8.2. *We have the following generating series of the dimensions of* $\mathcal{S}^{\text{new}}_k(\Gamma_1(N))^{\pm}$ *for* $N = 2, 3$*:*

$$\sum_{k=6}^{\infty} \dim(\mathcal{S}^{\text{new}}_k(\Gamma_1(2))^+) x^k = \frac{x^8}{(1-x^6)(1-x^8)}, \tag{8.8.1}$$

$$\sum_{k=6}^{\infty} \dim(\mathcal{S}^{\text{new}}_k(\Gamma_1(2))^-) x^k = \frac{x^2(1+x^{18})}{(1-x^8)(1-x^{12})}, \tag{8.8.2}$$

$$\sum_{k=6}^{\infty} \dim(\mathcal{S}^{\text{new}}_k(\Gamma_1(3))^+) x^k = \frac{x^8}{(1-x^2)(1-x^{12})}, \tag{8.8.3}$$

$$\sum_{k=6}^{\infty} \dim(\mathcal{S}^{\text{new}}_k(\Gamma_1(3))^-) x^k = \frac{x^6(1+x^8+x^{10}-x^{12})}{(1-x^4)(1-x^{12})}. \tag{8.8.4}$$

Here I will state how to get Conjecture F from the proof of Theorem 8.4.3 in the case of $N = 2$. The reason for the case of $N = 3$ is exactly the same. In the proof of Theorem 8.4.3, we saw that for any restricted homogeneous even polynomial $p(x, y)$

of degree $k-2$, we have

$$\cdot\,(\mathcal{D}_{k,2}^2 \cdot \mathcal{C}_{k,2}^2) : p(x,y) \mapsto -p(y,x) - p(y,x+y) + p(x,x+y) + p\left(\frac{y}{2},x\right). \quad (8.8.5)$$

Let $\varepsilon = \pm 1$. The corresponding vector of $p(x,y)$ is an eigenvector with eigenvalue $-1-\frac{\varepsilon}{2^{\frac{k-2}{2}}}$ if and only if we have

$$-p(y,x) - p(y,x+y) + p(x,x+y) + p\left(\frac{y}{2},x\right) = \left(-1-\frac{\varepsilon}{2^{\frac{k-2}{2}}}\right)p(x,y). \quad (8.8.6)$$

Lemma 8.8.3. *Let $\varepsilon = \pm 1$. A restricted homogeneous even polynomial $p(x,y)$ of degree $k-2$ satisfies (8.8.6) if and only if it satisfies both of the following equations:*

$$\begin{aligned} -p(y,x) - p(y,x+y) + p(x,x+y) &= -p(x,y) && (8.8.7)\\ p(y,2x) &= -\varepsilon \cdot 2^{\frac{k-2}{2}} p(x,y). && (8.8.8) \end{aligned}$$

Proof of Lemma 8.8.3. It is clear that equations (8.8.7) and (8.8.8) imply (8.8.6). So we only need to prove the opposite direction. If we have (8.8.6), then by the change-of-variables $x \mapsto y$ and $y \mapsto x$, we get

$$\begin{aligned} -p(y,x) - p(y,x+y) + p(x,x+y) + p\left(\frac{y}{2},x\right) &= \left(-1-\frac{\varepsilon}{2^{\frac{k-2}{2}}}\right)p(x,y),\\ -p(x,y) - p(x,x+y) + p(y,x+y) + p\left(\frac{x}{2},y\right) &= \left(-1-\frac{\varepsilon}{2^{\frac{k-2}{2}}}\right)p(y,x). \quad (8.8.9) \end{aligned}$$

Summing up (8.8.6) and (8.8.9), we get

$$p\left(\frac{y}{2},x\right) + p\left(\frac{x}{2},y\right) = -\frac{\varepsilon}{2^{\frac{k-2}{2}}}\Big(p(x,y) + p(y,x)\Big) \quad (8.8.10)$$

Letting $x \mapsto 2x$ and $y \mapsto 2y$ in (8.8.10), we have

$$p(y,2x) + p(x,2y) = -\varepsilon \cdot 2^{\frac{k-2}{2}}\Big(p(x,y) + p(y,x)\Big) \quad (8.8.11)$$

Now assume that $p(x, y)$ has the following expression

$$p(x,y) = \sum_{n=2:\text{even}}^{k-4} a_n x^n y^{k-2-n}.$$

Then

$$\begin{aligned}
\text{LHS of (8.8.11)} &= p(y,2x) + p(x,2y) \\
&= \sum_{n=2:\text{even}}^{k-4} a_n y^n (2x)^{k-2-n} + \sum_{n=2:\text{even}}^{k-4} a_n x^n (2y)^{k-2-n} \\
&= \sum_{n=2:\text{even}}^{k-4} (a_{k-2-n} 2^n + a_n 2^{k-2-n}) x^n y^{k-2-n}, \qquad (8.8.12) \\
\text{RHS of (8.8.11)} &= -\varepsilon \cdot 2^{\frac{k-2}{2}} \Big(p(x,y) + p(y,x) \Big) \\
&= \sum_{n=2:\text{even}}^{k-4} (-\varepsilon \cdot 2^{\frac{k-2}{2}} a_n + -\varepsilon \cdot 2^{\frac{k-2}{2}} a_{k-2-n}) x^n y^{k-2-n} \qquad (8.8.13)
\end{aligned}$$

Comparing (8.8.12) with (8.8.13), for any even n between 2 and $k-4$, we have

$$\begin{aligned}
& a_{k-2-n} 2^n + a_n 2^{k-2-n} = -\varepsilon \cdot 2^{\frac{k-2}{2}} a_n + -\varepsilon \cdot 2^{\frac{k-2}{2}} a_{k-2-n} \\
\Longleftrightarrow\ & (2^{k-2-n} + \varepsilon 2^{\frac{k-2}{2}}) a_n = -(2^n + \varepsilon 2^{\frac{k-2}{2}}) a_{k-2-n} \\
\Longleftrightarrow\ & 2^{\frac{k-2}{2}} (2^{\frac{k-2}{2}-n} + \varepsilon) a_n = -\varepsilon \cdot 2^n (\varepsilon + 2^{\frac{k-2}{2}-n}) a_{k-2-n} \\
\Longleftrightarrow\ & 2^{\frac{k-2}{2}} a_n = -\varepsilon \cdot 2^n a_{k-2-n} \\
\Longleftrightarrow\ & a_{k-2-n} 2^n = -\varepsilon \cdot 2^{\frac{k-2}{2}} a_n
\end{aligned}$$

Hence (8.8.11) is equivalent to

$$p(y,2x) = -\varepsilon \cdot 2^{\frac{k-2}{2}} p(x,y),$$

which is exactly (8.8.8). Now by the change-of-variables $x \mapsto \frac{x}{2}$ and $y \mapsto \frac{y}{2}$ in (8.8.8), (8.8.6) also implies that

$$p\left(\frac{y}{2}, x\right) = -\frac{\varepsilon}{2^{\frac{k-2}{2}}} p(x,y). \qquad (8.8.14)$$

Subtracting (8.8.14) from (8.8.6), we get (8.8.7). □

Remark. A similar result can be shown for the level $N = 3$ case, and we will not provide the proof here. The two equations in level $N = 3$ case are exactly the two equations that show up in the following conjecture.

The above Lemma 8.8.3 and the corresponding one for level $N = 3$ suggest the following conjecture.

Conjecture 8.8.4 (Eichler-Shimura-Manin correspondence for $\mathcal{S}_k^{\text{new}}(\Gamma_1(2))^{\pm}$ and $\mathcal{S}_k^{\text{new}}(\Gamma_1(3))^{\pm}$). *We have the following isomorphisms defined over* $\mathbb{C}$*:*

$$\mathcal{S}_k^{\text{new}}(\Gamma_1(2))^{\pm} \cong (\mathbf{W}_{2,\text{new}}^{-,0})^{\pm} := \left\{ p(x,y) \in \mathbb{C}[x,y] \;\middle|\; \begin{array}{l} 1)\;\; -p(y,x)-p(y,x+y)+p(x,x+y)=-p(x,y) \\ 2)\;\; -p(y,2x)=\pm 2^{\frac{k-2}{2}}p(x,y) \end{array} \right\},$$

$$\mathcal{S}_k^{\text{new}}(\Gamma_1(3))^{\pm} \cong (\mathbf{W}_{3,\text{new}}^{-,0})^{\pm} := \left\{ p(x,y) \in \mathbb{C}[x,y] \;\middle|\; \begin{array}{l} 1)\;\; -p(y,x)-p(y,x+y)+p(x,x+y) \\ \quad\;\; -p(y,x-y)+p(x,x-y)=-p(x,y) \\ 2)\;\; -p(y,3x)=\pm 3^{\frac{k-2}{2}}p(x,y) \end{array} \right\}.$$

This above conjecture is equivalent to the statement that the left eigenspaces of $\mathcal{D}_{k,2}^N \cdot \mathcal{C}_{k,2}^N$ with given eigenvalues as stated in Theorem 8.4.3 exactly consist of the restricted even period polynomials of newforms of level $\Gamma_1(N)$ and Atkin-Lehner eigenvalue ε.

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