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A Study on Multiple Zeta Values Related to Periods of Elliptic Modular Forms

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Contents

1 Introduction

In this paper, we will be interested in the multiple zeta value (MZV) related to modular forms (or their period polynomials) on the full modular group $\Gamma_1 = \mathrm{PSL}_2(\mathbb{Z})$ and its subgroup $\Gamma_0(2)$. This paper begins by studying an integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ defined by

$$\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}} = \delta_{(s_1,\dots,s_r),(k_1,\dots,k_r)} + \sum_{i=1}^{r-1} \delta_{(\hat{s}_1,\dots,\hat{s}_{i+1},\dots,s_r),(k_1,\dots,\hat{k}_i,\hat{k}_{i+1},\dots,k_r)} C^{s_1}_{k_i,k_{i+1}} \quad (s_i, k_i \in \mathbb{Z}_{>0}),$$

where $C^{s_1}_{k_i,k_{i+1}} = (-1)^{k_i}\binom{s_1-1}{k_i-1} + (-1)^{k_{i+1}-s_1}\binom{s_1-1}{k_{i+1}-1}$ and $\delta_{(s_1,\dots,s_r),(k_1,\dots,k_r)}$ is 1 if $s_i = k_i$ for all i, and 0 otherwise. In the case of $r = 2$, it is known that the integer $\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}$ is characterized by three different objects: even period polynomials, the Ihara action, and double Eisenstein series. The first main results of this paper (stated in Section 2) describe their generalizations: we show that there is an injective linear map from a certain vector space closely related to even period polynomials to the kernel of the matrix $\mathcal{E}_{k,r}$, whose entries are the above integers, and relate the integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ with polynomial representations of the Ihara action developed by Brown [3], and with the Fourier coefficients of the multiple Eisenstein series.

This work is mostly motivated by Brown's conjecture [3, Conjecture 5]. It is as follows. Throughout this paper, the MZV is defined by

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

for $\mathbf{k} = (k_1,\dots,k_r) \in \mathbb{Z}^r_{>0}$ with $k_r \geq 2$. We call $k_1 + \cdots + k_r$ ($=: \mathrm{wt}(\mathbf{k})$) the weight and r ($=: \mathrm{dep}(\mathbf{k})$) the depth. Let $\mathcal{Z}^{(r)}_k$ be the $\mathbb{Q}$-vector space spanned by all MZV of weight k and depth less than or equal to r, and $(\zeta(2))$ the ideal generated by $\zeta(2)$ in the MZV algebra $\mathcal{Z} = \bigoplus_{k\geq 0} \mathcal{Z}_k$, where $\mathcal{Z}_0 = \mathbb{Q}$ and $\mathcal{Z}_k = \mathcal{Z}^{(k-1)}_k$. We denote by $\mathcal{Z}_{k,r}$ the quotient vector space $\mathcal{Z}^{(r)}_k / \big(\mathcal{Z}^{(r-1)}_k + \mathcal{Z}^{(r)}_k \cap (\zeta(2))\big)$ and $\zeta_{\mathfrak{D}}(\mathbf{k})$ the equivalence class of the MZV $\zeta(\mathbf{k})$ of weight k and depth r in $\mathcal{Z}_{k,r}$. When all k_i are odd (≥ 3), we call $\zeta_{\mathfrak{D}}(k_1,\dots,k_r)$ the totally odd MZV. The $\mathbb{Q}$-vector subspace of $\mathcal{Z}_{k,r}$ spanned by all totally odd MZVs of weight k and depth r is denoted by

$$\mathcal{Z}^{\mathrm{odd}}_{k,r} = \big\langle \zeta_{\mathfrak{D}}(k_1,\dots,k_r) \in \mathcal{Z}_{k,r} \mid k_i \geq 3 : \mathrm{odd} \big\rangle_{\mathbb{Q}}.$$

Conjecture 1.1. ([3, Conjecture 5]) *The generating function of the dimension of the* *space* $\mathcal{Z}_{k,r}^{\mathrm{odd}}$ *is given by*

$$1+\sum_{k>r>0}\dim_{\mathbb{Q}}\mathcal{Z}_{k,r}^{\mathrm{odd}}x^k y^r \overset{?}{=} \frac{1}{1-\mathbb{O}(x)y+\mathbb{S}(x)y^2},$$

where $\mathbb{O}(x)=\frac{x^3}{1-x^2}=x^3+x^5+x^7+\cdots$, *and* $\mathbb{S}(x)=\frac{x^{12}}{(1-x^4)(1-x^6)}=x^{12}+x^{16}+x^{18}+\cdots$.

We note that the coefficient of x^k in $\mathbb{S}(x)$ coincides with the dimension of the space of cusp forms of weight k on Γ_1, and the coefficient of x^k in $\mathbb{O}(x)^r$ gives a trivial upper bound of the dimension of the space $\mathcal{Z}_{k,r}^{\mathrm{odd}}$, i.e. $|S_{k,r}|$. The power series expansion of the above $(1-\mathbb{O}(x)y+\mathbb{S}(x)y^2)^{-1}$ at $y=0$ is given by

$$\begin{aligned}\frac{1}{1-\mathbb{O}(x)y+\mathbb{S}(x)y^2} =& 1+\mathbb{O}(x)y+\big(\mathbb{O}(x)^2-\mathbb{S}(x)\big)y^2+\big(\mathbb{O}(x)^3-2\mathbb{O}(x)\mathbb{S}(x)\big)y^3\\ &+\big(\mathbb{O}(x)^4-3\mathbb{O}(x)^2\mathbb{S}(x)+\mathbb{S}(x)^2\big)y^4+\cdots.\end{aligned} \tag{1.1}$$

Hence, Conjecture 1.1 suggests that there are $\mathbb{Q}$-linear relations among totally odd MZVs related to cusp forms. For this conjecture, we have inequalities

$$\sum_{k>0}\dim_{\mathbb{Q}}\mathcal{Z}_{k,2}^{\mathrm{odd}}x^k \le \mathbb{O}(x)^2-\mathbb{S}(x) \quad \text{and} \quad \sum_{k>0}\dim_{\mathbb{Q}}\mathcal{Z}_{k,3}^{\mathrm{odd}}x^k \le \mathbb{O}(x)^3-2\mathbb{O}(x)\mathbb{S}(x),$$

which follow from results obtained by Goncharov [7, Theorems 2.4 and 2.5]. (Furthermore, we can find explicit relations when $r=2$, which is a result of Gangl-Kaneko-Zagier [6].) Here the notation $\sum_{k>0}a_kx^k \le \sum_{k>0}b_kx^k$ means $a_k \le b_k$ for all $k>0$.

The second main result of this paper is that the dimension of the space $\mathcal{Z}_{k,4}^{\mathrm{odd}}$ does not exceed the coefficient of x^ky^4 in the power series expansion of the right-hand side of (1.1).

Theorem 1.2. *We have*

$$\sum_{k>0}\dim\mathcal{Z}_{k,4}^{\mathrm{odd}}x^k \le \mathbb{O}(x)^4-3\mathbb{O}(x)^2\mathbb{S}(x)+\mathbb{S}(x)^2.$$

The third main results of this paper (described in Section 4) are concerned with the double Eisenstein series for $\Gamma_0(2)$. These studies are originated in the previous work of Gangl, Kaneko and Zagier [6]. We will start with showing the double shuffle relation, which is satisfied by the double zeta values of level 2 (Euler sums), for the double Eisenstein series on $\Gamma_0(2)$ (Theorem 4.2 and 4.13), and investigating the formal double shuffle space of level 2 (Theorem 4.3). These results have applications in not only double zeta values of level 2 but also modular forms on $\Gamma_0(2)$: for example, for even $k \geq 4$, we will prove that

$$\dim \left\langle \sum_{\substack{m>n>0 \\ m,n:\text{odd}}} \frac{1}{m^{2r} n^{k-2r}} \in \mathbb{R} \;\middle|\; 1 \leq r \leq k/2-1 \right\rangle_{\mathbb{Q}} \leq k/2 - 1 - \dim S_k(2)$$

(Corollary 4.7), and any modular form of weight k on $\Gamma_0(2)$ can be written as a linear combination of the Eisenstein series on $\Gamma_0(2)$ and its product (Theorem 4.8). Furthermore, we will show that the $8s$ power of the standard theta function $\theta(q) = \sum_{n\in\mathbb{Z}} q^{n^2}$ can be expressed uniquely as the sum of two products of the Eisenstein series on $\Gamma_0(2)$ for the cusp ∞ (Theorem 4.10), as conjectured by Chan and Chua [5].

The contents of this paper are as follows. In Section 2, we introduce the results concerning the integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$, which are used in Section 3 to prove Theorem 1.2. Section 4 is devoted to the study of the double Eisenstein series for $\Gamma_0(2)$. In the final section, we develop a connection between the integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ and period polynomials for $\Gamma_0(2)$, and give some observations on the "almost totally odd" MZVs.

2 Main results

Throughout the paper, the integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ defined by the formula

$$\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}} = \delta_{(s_1,\dots,s_r),(k_1,\dots,k_r)} + \sum_{i=1}^{r-1} \delta_{(\hat{s}_1,\dots,\hat{s}_{i+1},\dots,s_r),(k_1,\dots,\hat{k}_i,\hat{k}_{i+1},\dots,k_r)} C^{s_1}_{k_i,k_{i+1}} \tag{2.1}$$

plays an important role. Here, we define the Kronecker delta $\delta_{(s_1,\dots,s_r),(k_1,\dots,k_r)}$ by

$$\delta_{(s_1,\dots,s_r),(k_1,\dots,k_r)} = \begin{cases} 1 & \text{if } s_i = k_i \text{ for all } i \in \{1,\dots,r\} \\ 0 & \text{otherwise} \end{cases},$$

and the integer $C^s_{k,k'}$ for $s,k,k' \geq 1$ by

$$C^s_{k,k'} = (-1)^k \binom{s-1}{k-1} + (-1)^{k'-s} \binom{s-1}{k'-1}.$$

(Note $(s_1,\dots,\hat{s}_i,\dots,s_r)=(s_1,\dots,s_{i-1},s_{i+1},\dots,s_r)$.) The integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ appears in connection with period polynomials, linear relations among totally odd MZVs, and the Fourier coefficients of multiple Eisenstein series. Our goal of this section is to describe these connections.

2.1 Connection with restricted even period polynomials

Let $S_{k,r}$ be the set of totally odd indices of weight k and depth r:

$$S_{k,r}=\{(k_1,\dots,k_r)\in\mathbb{Z}_{>0}\mid k_1+\cdots+k_r=k,\ k_i\geq 3:\mathrm{odd}\}.$$

Consider the $|S_{k,r}|\times|S_{k,r}|$ matrix

$$\mathcal{E}_{k,r}=\left(\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}\right)_{\substack{(s_1,\dots,s_r)\in S_{k,r}\\(k_1,\dots,k_r)\in S_{k,r}}}$$

whose rows and columns are indexed by $(s_1,\dots,s_r)$ and $(k_1,\dots,k_r)$ in the set $S_{k,r}$ respectively. Baumard and Schneps [4] showed that there is a one to one correspondence between the space of restricted even period polynomials and the left kernel of the matrix $\mathcal{E}_{k,2}$. For $r\geq 3$, we see below that there is an injective map from a certain vector space closely related to restricted even period polynomials to the left kernel of $\mathcal{E}_{k,r}$.

We begin with reviewing and reproving the result obtained by Baumard and Schneps. Let $V_k=\langle x_1^{s_1-1}x_2^{s_2-1}\mid(s_1,s_2)\in S_{k,2}\rangle_{\mathbb{Q}}$ and

$$W_k^{-,0}=\big\{p(x_1,x_2)\in V_k\mid p(x_1,x_2)=p(x_2-x_1,x_2)-p(x_2-x_1,x_1)\big\}.$$

This space is called the space of restricted even period polynomials. We only use the fact, known as the Eichler-Shimura-Manin correspondence, that $W_k^{-,0}\otimes_{\mathbb{Q}}\mathbb{C}\cong S_k(\Gamma_1)$, and hence

$$\dim W_k^{-,0}=\dim S_k(\Gamma_1)\tag{2.2}$$

(see [6, 10, 11] for the detail). Here, the space $S_k(\Gamma_1)$ is the $\mathbb{C}$-vector space of cusp forms of weight k on Γ_1. Baumard and Schneps showed the following:

Proposition 2.1. ([4, Proposition 3.2]) *Let $(a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}}$ be a row vector with rational coefficients. Then the following assertions are equivalent.*

(i) The vector $(a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}}$ is a left annihilator of the matrix $\mathcal{E}_{k,2}$.
(ii) The polynomial $\sum_{(s_1,s_2)\in S_{k,2}} a_{s_1,s_2} x_1^{s_1-1}x_2^{s_2-1}$ is an element of the space $W_k^{-,0}$.

Proof. For a polynomial $p(x_1,x_2)=\sum_{(s_1,s_2)\in S_{k,2}} a_{s_1,s_2} x_1^{s_1-1}x_2^{s_2-1}$ satisfying $p(x,x)=0$, one can compute

$$\begin{aligned}
&p(x_1,x_2)-p(x_2-x_1,x_2)+p(x_2-x_1,x_1)\\
&=\sum_{\substack{k_1+k_2=k\\k_1,k_2\geq 2}}\Bigg(\sum_{(s_1,s_2)\in S_{k,2}} a_{s_1,s_2}\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}\Bigg)x_1^{k_1-1}x_2^{k_2-1}\\
&=\sum_{(k_1,k_2)\in S_{k,2}}\Bigg(\sum_{(s_1,s_2)\in S_{k,2}} a_{s_1,s_2}\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}\Bigg)x_1^{k_1-1}x_2^{k_2-1} &(2.3)\\
&+\frac{1}{2}\big(p(x_2-x_1,x_1)-p(x_2-x_1,x_2)-p(x_2+x_1,x_1)+p(x_2+x_1,x_2)\big). &(2.4)
\end{aligned}$$

Assuming (ii), from $p(x_1,x_2)=p(x_2+x_1,x_2)-p(x_2+x_1,x_1)$, we have (2.4)$=0$, and then (2.3)$=0$. This gives the assertion (i). To prove (i)$\Rightarrow$(ii), we use the action of the group $\mathrm{PGL}_2(\mathbb{Z})$ on V_k defined by $(f\big|\gamma)(x_1,x_2)=f(ax_1+bx_2,cx_1+dx_2)$ for $\gamma=\left(\begin{smallmatrix}a&b\\c&d\end{smallmatrix}\right)$ and $f\in V_k$. Set

$$\delta=\begin{pmatrix}-1&0\\0&1\end{pmatrix},\ \varepsilon=\begin{pmatrix}0&1\\1&0\end{pmatrix},\ T=\begin{pmatrix}1&1\\0&1\end{pmatrix}.$$

For the left annihilator $(a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}}$ of $\mathcal{E}_{k,2}$, putting $p(x_1,x_2)=\sum_{(s_1,s_2)\in S_{k,2}} a_{s_1,s_2} x_1^{s_1-1}x_2^{s_2-1}$, one easily finds that $p\big|(\varepsilon+1)=0$ and $p\big|(\delta-1)=0$, where we have extended the action of $\mathrm{PGL}_2(\mathbb{Z})$ to its group ring by linearity. Using $T\delta=\delta T^{-1}$ and $T\varepsilon\delta=\varepsilon T\varepsilon T^{-1}$, we have $p\big|(1-T+T\varepsilon)\delta=p\big|(1-T^{-1}+\varepsilon T\varepsilon T^{-1})=-p\big|(1-T+T\varepsilon)T^{-1}$. Let $G=p\big|(1-T+T\varepsilon)$. Then we find that $G(0,x_2)=0$ and

$$\begin{aligned}
0&=2\times(2.3)=2\times(p(x_1,x_2)-p(x_2-x_1,x_2)+p(x_2-x_1,x_1))-2\times(2.4)\\
&=G\big|(1+\delta)=G\big|(1-T^{-1}),
\end{aligned}$$

which implies $G=0$. The assertion follows from

$$\begin{aligned}
0=&G(x_1,x_2)=p(x_1,x_2)-p(x_2+x_1,x_2)+p(x_2+x_1,x_1)\\
=&p(x_1,x_2)-p(x_2-x_1,x_2)+p(x_2-x_1,x_1).
\end{aligned}$$

$\square$

Corollary 2.2. *Let us denote by* $\ker \mathcal{E}_{k,2}$ *the* $\mathbb{Q}$*-vector space spanned by all left annihilators of the matrix* $\mathcal{E}_{k,2}$*. Then, for each integer* k*, we have*

$$\dim \ker \mathcal{E}_{k,2} = \dim S_k(\Gamma_1), \tag{2.5}$$

or equivalently, $\operatorname{rank} \mathcal{E}_{k,2} = |S_{k,2}| - \dim S_k(\Gamma_1)$.

Proof. This follows immediately from (2.2) and Proposition 2.1. □

We now turn to the result in the case of depth greater than 2. Let $\mathcal{V}_{k,r}$ be the $|S_{k,r}|$-dimensional vector space over $\mathbb{Q}$ spanned by the set of row vectors $(a_{s_1,\ldots,s_r})_{(s_1,\ldots,s_r)\in S_{k,r}}$:

$$\mathcal{V}_{k,r} = \{(\ldots, a_{s_1,\ldots,s_r}, \ldots)_{(s_1,\ldots,s_r)\in S_{k,r}} \mid a_{s_1,\ldots,s_r} \in \mathbb{Q}\}.$$

Hereafter, we identify the matrix $A \in M_{|S_{k,r}|}(\mathbb{Z})$ with its induced linear map $A : \mathcal{V}_{k,r} \to \mathcal{V}_{k,r}, v \mapsto A(v) := v \cdot A$, and denote by $\ker A$ the $\mathbb{Q}$-vector subspace of $\mathcal{V}_{k,r}$ spanned by all left annihilators of the matrix A. For $i \in \{1, \ldots, r-1\}$, let us denote by $\varepsilon^{(i)}_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$ the i-th part of $\varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$ in (2.1) and $\mathfrak{E}^{(i)}_{k,r}$ the $|S_{k,r}| \times |S_{k,r}|$ matrix whose entries are the integers $\varepsilon^{(i)}_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$, so that

$$\varepsilon^{(i)}_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}} = \delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,\ldots,\hat{k}_i,\hat{k}_{i+1},\ldots,k_r)} C^{s_1}_{k_i,k_{i+1}}, \;\; \mathfrak{E}^{(i)}_{k,r} = \left(\varepsilon^{(i)}_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}\right)_{\substack{(s_1,\ldots,s_r)\in S_{k,r} \\ (k_1,\ldots,k_r)\in S_{k,r}}}.$$

Denote by $\mathcal{W}_{k,r}$ the $\mathbb{Q}$-vector subspace of $\mathcal{V}_{k,r}$ spanned by all left annihilators of the matrix $I + \mathfrak{E}^{(1)}_{k,r}$:

$$\mathcal{W}_{k,r} = \ker\big(I + \mathfrak{E}^{(1)}_{k,r}\big),$$

where I is the identity matrix $\big(\delta_{(s_1,\ldots,s_r),(k_1,\ldots,k_r)}\big)$ in $M_{|S_{k,r}|}(\mathbb{Z})$. For $(k_1, \ldots, k_r) \in S_{k,r}$, the $(k_1, \ldots, k_r)$-th entry of the vector $(a_{s_1,\ldots,s_r})_{(s_1,\ldots,s_r)\in S_{k,r}} \cdot \big(I + \mathfrak{E}^{(1)}_{k,r}\big)$ is given by

$$\begin{aligned} &\sum_{(s_1,\ldots,s_r)\in S_{k,r}} a_{s_1,\ldots,s_r} \big(\delta_{(s_1,\ldots,s_r),(k_1,\ldots,k_r)} + \delta_{(s_3,\ldots,s_r),(k_3,\ldots,k_r)} C^{s_1}_{k_1,k_2}\big) \\ &= \sum_{(s_1,\ldots,s_r)\in S_{k,r}} a_{s_1,\ldots,s_r} \varepsilon_{\binom{s_1,s_2}{k_1,k_2}} \delta_{(s_3,\ldots,s_r),(k_3,\ldots,k_r)} = \sum_{(s_1,s_2)\in S_{k-p,2}} a_{s_1,s_2,k_3,\ldots,k_r} \varepsilon_{\binom{s_1,s_2}{k_1,k_2}}, \end{aligned}$$

where $p = k_3 + \cdots + k_r$. Hence, we find that the space $\mathcal{W}_{k,r}$ splits as the direct sum in the form

$$\mathcal{W}_{k,r} = \bigoplus_{\substack{0<p<k \\ (k_3,\dots,k_r)\in S_{p,r-2}}} \Big\langle \big(a_{s_1,s_2}\delta_{(k_3,\dots,k_r),(s_3,\dots,s_r)}\big)_{(s_1,\dots,s_r)\in S_{k,r}} \,\Big|\, (a_{s_1,s_2})_{(s_1,s_2)\in S_{k-p,2}} \in \mathcal{W}_{k-p,2} \Big\rangle_{\mathbb{Q}}. \tag{2.6}$$

We also find $\mathcal{W}_{k,2} = \ker \mathcal{E}_{k,2}$, which gives $\dim \mathcal{W}_{k,2} = \dim S_k(\Gamma_1)$ (Corollary 2.2). Thus, by (2.6), one can obtain the dimension of the space $\mathcal{W}_{k,r}$ as follows:

$$\sum_{k>0} \dim \mathcal{W}_{k,r} x^k = \mathbb{O}(x)^{r-2}\mathbb{S}(x). \tag{2.7}$$

Here recall that $\mathbb{O}(x)^r = \sum_{k>0} |S_{k,r}| x^k$ and $\mathbb{S}(x) = \sum_{k>0} \dim S_k(\Gamma_1)x^k$. We now prove that there is an injective linear map from $\mathcal{W}_{k,r}$ to $\ker \mathcal{E}_{k,r}$.

Theorem 2.3. *Let r be a positive integer greater than 2 and $\mathcal{F}_{k,r}$ the matrix $\mathfrak{E}_{k,r}^{(1)} + \cdots + \mathfrak{E}_{k,r}^{(r-1)} (= \mathcal{E}_{k,r} - I)$. Then, for any $v \in \mathcal{W}_{k,r}$, we have $(v \cdot \mathcal{F}_{k,r}) \cdot \mathcal{E}_{k,r} = 0$. Furthermore, the map $\mathcal{F}_{k,r}$ is an injective map from $\mathcal{W}_{k,r}$ to $\ker \mathcal{E}_{k,r}$, which from* (2.7) *entails*

$$\sum_{k>0} \dim \ker \mathcal{E}_{k,r} x^k \geq \mathbb{O}(x)^{r-2}\mathbb{S}(x). \tag{2.8}$$

Proof. Consider the action $E_r^{(i)}$ on $V_{k,r} := \langle x_1^{s_1-1}\cdots x_r^{s_r-1} \mid (s_1,\dots,s_r) \in S_{k,r}\rangle_{\mathbb{Q}}$ defined by

$$f(x_1,\dots,k_r)\big|E_r^{(i)} = f(x_{i+1}-x_i, x_1,\dots,\hat{x}_{i+1},\dots,x_r) - f(x_{i+1}-x_i, x_1,\dots,\hat{x}_i,\dots,x_r)$$

for $f(x_1,\dots,x_r) \in V_{k,r}$. For each $v = (a_{s_1,\dots,s_r})_{(s_1,\dots,s_r)\in S_{k,r}} \in \mathcal{W}_{k,r}$, writing $p(x_1,\dots,x_r) = \sum_{(s_1,\dots,s_r)\in S_{k,r}} a_{s_1,\dots,s_r} x_1^{s_1-1}\cdots x_r^{s_r-1}$, we have

$$\begin{aligned} &p(x_1,\dots,x_r) - p(x_2-x_1, x_2, x_3,\dots,x_r) + p(x_2-x_1, x_1, x_3,\dots,x_r) \\ &= \sum_{(s_1,\dots,s_r)\in S_{k,r}} a_{s_1,\dots,s_r} \sum_{k_1+\cdots+k_r=k} \big(\varepsilon_{\binom{s_1,s_2}{k_1,k_2}} \delta_{(s_3,\dots,s_r),(k_3,\dots,k_r)}\big) x_1^{k_1-1}\cdots x_r^{k_r-1} \\ &=0, \end{aligned} \tag{2.9}$$

because of Proposition 2.1. We now prove

$$p(x_1,\dots,x_r)\big|(E_r^{(j)}E_r^{(i)} + E_r^{(i)}E_r^{(j-1)}) = 0 \quad (r-1 \geq i \geq j \geq 2). \tag{2.10}$$

For $r-1 \geq i > j \geq 2$ we can check

$$
\begin{aligned}
& p(x_1,\ldots,x_r)\big|(E_r^{(j)}E_r^{(i)} + E_r^{(i)}E_r^{(j-1)}) \\
& = p(x_j - x_{j-1}, x_{i+1} - x_i, x_1, \ldots, \hat{x}_j, \ldots, \hat{x}_{i+1}, \ldots, x_r) \\
& - p(x_j - x_{j-1}, x_{i+1} - x_i, x_1, \ldots, \hat{x}_{j-1}, \ldots, \hat{x}_{i+1}, \ldots, x_r) \\
& - p(x_j - x_{j-1}, x_{i+1} - x_i, x_1, \ldots, \hat{x}_j, \ldots, \hat{x}_i, \ldots, x_r) \\
& + p(x_j - x_{j-1}, x_{i+1} - x_i, x_1, \ldots, \hat{x}_{j-1}, \ldots, \hat{x}_i, \ldots, x_r) \\
& + p(x_{i+1} - x_i, x_j - x_{j-1}, x_1, \ldots, \hat{x}_j, \ldots, \hat{x}_{i+1}, \ldots, x_r) \\
& - p(x_{i+1} - x_i, x_j - x_{j-1}, x_1, \ldots, \hat{x}_j, \ldots, \hat{x}_i, \ldots, x_r) \\
& - p(x_{i+1} - x_i, x_j - x_{j-1}, x_1, \ldots, \hat{x}_{j-1}, \ldots, \hat{x}_{i+1}, \ldots, x_r) \\
& + p(x_{i+1} - x_i, x_j - x_{j-1}, x_1, \ldots, \hat{x}_{j-1}, \ldots, \hat{x}_i, \ldots, x_r) \\
& = 0
\end{aligned}
$$

by using $p(x_1, x_2, x_3, \ldots, x_r) + p(x_2, x_1, x_3, \ldots, x_r) = 0$, and for $r-1 \geq i = j \geq 2$ we have

$$
\begin{aligned}
& p(x_1,\ldots,x_r)\big|(E_r^{(j)}E_r^{(j)} + E_r^{(j)}E_r^{(j-1)}) \\
& = p(x_j - x_{j-1}, x_{j+1} - x_j, x_1, \ldots, \hat{x}_j, \hat{x}_{j+1}, \ldots, x_r) \\
& - p(x_j - x_{j-1}, x_{j+1} - x_j, x_1, \ldots, \hat{x}_{j-1}, x_j, \hat{x}_{j+1}, \ldots, x_r) \\
& - p(x_j - x_{j-1}, x_{j+1} - x_j, x_1, \ldots, \hat{x}_j, \hat{x}_{j+1}, \ldots, x_r) \\
& + p(x_j - x_{j-1}, x_{j+1} - x_j, x_1, \ldots, \hat{x}_{j-1}, \hat{x}_j, \ldots, x_r) \\
& + p(x_{j+1} - x_{j-1}, x_j - x_{j-1}, x_1, \ldots, \hat{x}_j, \hat{x}_{j+1}, \ldots, x_r) \\
& - p(x_{j+1} - x_{j-1}, x_j - x_{j-1}, x_1, \ldots, \hat{x}_{j-1}, \hat{x}_j, \ldots, x_r) \\
& - p(x_{j+1} - x_j, x_j - x_{j-1}, x_1, \ldots, \hat{x}_{j-1}, x_j, \hat{x}_{j+1}, \ldots, x_r) \\
& + p(x_{j+1} - x_j, x_j - x_{j-1}, x_1, \ldots, \hat{x}_{j-1}, \hat{x}_j, \ldots, x_r) \\
& = 0,
\end{aligned}
$$

where for the last equality we have used (2.9). A direct computation shows that, for any $(k_1, \ldots, k_r) \in S_{k,r}$, the $(k_1, \ldots, k_r)$-th entry of the vector $(a_{s_1,\ldots,s_r})_{(s_1,\ldots,s_r)\in S_{k,r}} \cdot$

$\mathfrak{E}_{k,r}^{(j)} \cdot \mathfrak{E}_{k,r}^{(i)} \in \mathcal{V}_{k,r}$ is given by the coefficient of $x_1^{k_1-1} \cdots x_r^{k_r-1}$ in

$$\begin{aligned}
&\sum_{(s_1,\dots,s_r)\in S_{k,r}} a_{s_1,\dots,s_r} x_1^{s_1-1} \cdots x_r^{s_r-1} \big| E_r^{(j)} \big| E_r^{(i)} \\
&= \sum_{k_1+\cdots+k_r=k} \left(\sum_{(s_1,\dots,s_r)\in S_{k,r}} a_{s_1,\dots,s_r} \sum_{t_1+\cdots+t_r=k} \varepsilon^{(j)}_{\binom{s_1,\dots,s_r}{t_1,\dots,t_r}} \varepsilon^{(i)}_{\binom{t_1,\dots,t_r}{k_1,\dots,k_r}} \right) x^{k_1-1} \cdots x_r^{k_r-1},
\end{aligned}$$

because, by the definition of $\varepsilon^{(i)}_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$, the product $\varepsilon^{(j)}_{\binom{s_1,\dots,s_r}{t_1,\dots,t_r}} \varepsilon^{(i)}_{\binom{t_1,\dots,t_r}{k_1,\dots,k_r}}$ is 0 if $(t_1,\dots,t_r) \notin S_{k,r}$. Combining this with (2.10), we obtain

$$v \cdot (\mathfrak{E}_{k,r}^{(j)} \mathfrak{E}_{k,r}^{(i)} + \mathfrak{E}_{k,r}^{(i)} \mathfrak{E}_{k,r}^{(j-1)}) = 0 \quad (r-1 \geq i \geq j \geq 2).$$

Then the first statement follows from

$$\begin{aligned}
(v \cdot \mathcal{F}_{k,r}) \cdot \mathcal{E}_{k,r} =& v \cdot (\mathfrak{E}_{k,r}^{(1)} + \cdots + \mathfrak{E}_{k,r}^{(r-1)}) \cdot (I + \mathfrak{E}_{k,r}^{(1)} + \cdots + \mathfrak{E}_{k,r}^{(r-1)}) \\
=& v \cdot (\mathfrak{E}_{k,r}^{(2)} + \cdots + \mathfrak{E}_{k,r}^{(r-1)}) \cdot (\mathfrak{E}_{k,r}^{(1)} + \cdots + \mathfrak{E}_{k,r}^{(r-1)}) \\
=& v \cdot \sum_{r-1 \geq i \geq j \geq 2} (\mathfrak{E}_{k,r}^{(j)} \mathfrak{E}_{k,r}^{(i)} + \mathfrak{E}_{k,r}^{(i)} \mathfrak{E}_{k,r}^{(j-1)}) \\
=& 0.
\end{aligned}$$

For the injectivity of the map $\mathcal{F}_{k,r}$, it suffices to check that

$$\mathcal{W}_{k,r} \cap \ker \mathcal{F}_{k,r} = 0.$$

Assume that $v = (a_{s_1,\dots,s_r})_{(s_1,\dots,s_r)\in S_{k,r}}$ is an element of $\mathcal{W}_{k,r} \cap \ker \mathcal{F}_{k,r}$. For each $(k_1,\dots,k_r) \in S_{k,r}$, the relation $\mathcal{F}_{k,r}(v) = 0$ gives

$$\sum_{(s_1,\dots,s_r)\in S_{k,r}} \Big(\sum_{i=1}^{r-1} \delta_{(\hat{s}_1,\dots,\hat{s}_{i+1},\dots,s_r),(k_1,\dots,\hat{k}_i,\hat{k}_{i+1},\dots,k_r)} C^{s_1}_{k_i,k_{i+1}} \Big) a_{s_1,\dots,s_r} = 0.$$

With this and the relation $(I + \mathfrak{E}_{k,r}^{(1)})(v) = 0$, we have

$$\sum_{(s_1,\dots,s_r)\in S_{k,r}} \Big(-\delta_{(s_1,\dots,s_r),(k_1,\dots,k_r)} + \sum_{i=2}^{r-1} \delta_{(\hat{s}_1,\dots,\hat{s}_{i+1},\dots,s_r),(k_1,\dots,\hat{k}_i,\hat{k}_{i+1},\dots,k_r)} C^{s_1}_{k_i,k_{i+1}} \Big) a_{s_1,\dots,s_r} = 0. \tag{2.11}$$

Furthermore, by (2.6), for any fixed index $(s_3, \ldots, s_r) \in S_{p,r-2}$ $(p = s_3 + \cdots + s_r)$, we see that the relation (2.11) can be computed as follows:

$$
\begin{aligned}
0 = &\sum_{(s_1,s_2)\in S_{k-p,2}} \Big(\delta_{(s_1,\ldots,s_r),(k_1,\ldots,k_r)} - \sum_{i=2}^{r-1} \delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,\ldots,\hat{k}_i,\hat{k}_{i+1},\ldots,k_r)} C^{s_1}_{k_i,k_{i+1}}\Big) a_{s_1,\ldots,s_r} \\
=&\delta_{(s_3,\ldots,s_r),(k_3,\ldots,k_r)} a_{k_1,k_2,k_3,\ldots,k_r} \\
&- \sum_{(s_1,s_2)\in S_{k-p,2}} \sum_{i=2}^{r-1} \delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,\ldots,\hat{k}_i,\hat{k}_{i+1},\ldots,k_r)} C^{s_1}_{k_i,k_{i+1}} a_{s_1,\ldots,s_r}.
\end{aligned}
$$

Denote by $\alpha(k_1, \ldots, k_r; s_3, \ldots, s_r)$ the right-hand side of the above equation and $\mathrm{bij}\{2, \ldots, r\}$ the set of all bijections on the set $\{2, \ldots, r\}$. Consider

$$
\begin{aligned}
&\mathfrak{f}(s_3, \ldots, s_r) := \sum_{\sigma\in \mathrm{bij}\{2,\ldots,r\}} \alpha(k_1, k_{\sigma(2)}, k_{\sigma(3)}, \ldots, k_{\sigma(r)}; s_3, \ldots, s_r) \\
&= \sum_{\sigma\in \mathrm{bij}\{2,\ldots,r\}} \delta_{(s_3,\ldots,s_r),(k_{\sigma(3)},\ldots,k_{\sigma(r)})} a_{k_1,k_{\sigma(2)},\ldots,k_{\sigma(r)}} \\
&- \sum_{(s_1,s_2)\in S_{k-p,2}} \sum_{i=2}^{r-1} \sum_{\sigma\in \mathrm{bij}\{2,\ldots,r\}} a_{s_1,\ldots,s_r} \Big(\delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,k_{\sigma(2)},\ldots,\hat{k}_{\sigma(i)},\hat{k}_{\sigma(i+1)},\ldots,k_{\sigma(r)})} C^{s_1}_{k_{\sigma(i)},k_{\sigma(i+1)}}\Big).
\end{aligned}
$$

Note that for each $\sigma \in \mathrm{bij}\{2, \ldots, r\}$ there exists a unique $\tau \in \mathrm{bij}\{2, \ldots, r\}$ such that $\sigma(j) = \tau(j)$ if $j \in \{2, \ldots, i-1, i+2, \ldots, r\}$ and $\sigma(i) = \tau(i+1)$, $\sigma(i+1) = \tau(i)$. For the above σ and τ, we have

$$
\begin{aligned}
a_{s_1,\ldots,s_r} \Big(&\delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,k_{\sigma(2)},\ldots,\hat{k}_{\sigma(i)},\hat{k}_{\sigma(i+1)},\ldots,k_{\sigma(r)})} C^{s_1}_{k_{\sigma(i)},k_{\sigma(i+1)}} \\
&+ \delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,k_{\tau(2)},\ldots,\hat{k}_{\tau(i)},\hat{k}_{\tau(i+1)},\ldots,k_{\tau(r)})} C^{s_1}_{k_{\tau(i)},k_{\tau(i+1)}}\Big) = 0,
\end{aligned}
$$

and hence for each $i \in \{2, \ldots, r-1\}$, we have

$$
\sum_{\sigma\in \mathrm{bij}\{2,\ldots,r\}} a_{s_1,\ldots,s_r} \Big(\delta_{(\hat{s}_1,\ldots,\hat{s}_{i+1},\ldots,s_r),(k_1,k_{\sigma(2)},\ldots,\hat{k}_{\sigma(i)},\hat{k}_{\sigma(i+1)},\ldots,k_{\sigma(r)})} C^{s_1}_{k_{\sigma(i)},k_{\sigma(i+1)}}\Big) = 0.
$$

We therefore have

$$
\mathfrak{f}(s_3, \ldots, s_r) = \sum_{\sigma\in \mathrm{bij}\{2,\ldots,r\}} \delta_{(s_3,\ldots,s_r),(k_{\sigma(3)},\ldots,k_{\sigma(r)})} a_{k_1,k_{\sigma(2)},\ldots,k_{\sigma(r)}}.
$$

Letting $s_i = k_i$ for all $i \in \{3, \ldots, r\}$, we obtain

$$\begin{aligned}
0 &= \mathfrak{f}(k_3, \ldots, k_r) \\
&= \sum_{\sigma \in \mathrm{bij}\{2,\ldots,r\}} \delta_{(k_3,\ldots,k_r),(k_{\sigma(3)},\ldots,k_{\sigma(r)})} a_{k_1,k_{\sigma(2)},\ldots,k_{\sigma(r)}} \\
&= \Big(\sum_{\sigma \in \mathrm{bij}\{2,\ldots,r\}} \delta_{(k_3,\ldots,k_r),(k_{\sigma(3)},\ldots,k_{\sigma(r)})} \Big) a_{k_1,\ldots,k_r},
\end{aligned}$$

which gives $a_{k_1,\ldots,k_r} = 0$ for all $(k_1, \ldots, k_r) \in S_{k,r}$. This completes the proof of Theorem 2.3. □

Remark. Conjecturally, the dimension of $\ker \mathcal{E}_{k,r}$ coincides with the coefficient of x^k in $\mathbb{O}(x)^{r-2}\mathbb{S}(x)$. Therefore, from (2.7) we may expect that $\mathcal{F}_{k,r}$ gives a bijection from $\mathcal{W}_{k,r}$ to $\ker \mathcal{E}_{k,r}$. We have a computational evidence up to $k = 35$ for this expectation.

2.2 Connection with linear relations among totally odd MZVs

The connection between the integer $\varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$ and linear relations among totally odd MZVs can be stated as follows:

Proposition 2.4. *For any right annihilator $(a_{k_1,\ldots,k_r})_{(k_1,\ldots,k_r)\in S_{k,r}}$ of the matrix $\mathcal{E}_{k,r}$, we have*

$$\sum_{(k_1,\ldots,k_r)\in S_{k,r}} a_{k_1,\ldots,k_r} \zeta_{\mathfrak{D}}(k_1, \ldots, k_r) = 0.$$

In the case of $r = 2$, Proposition 2.4 was first proved by Gangl, Kaneko and Zagier [6] by using double shuffle relations. Before we prove this, we illustrate a few examples of the relations. For $r = 2$, the matrix

$$\mathcal{E}_{12,2} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ -6 & 0 & 1 & 6 \\ -15 & -14 & 15 & 15 \\ -27 & -42 & 42 & 28 \end{pmatrix}$$

is annihilated by the vector ${}^t(14, 75, 84, 0)$. This gives the relation

$$14\zeta_{\mathfrak{D}}(3, 9) + 75\zeta_{\mathfrak{D}}(5, 7) + 84\zeta_{\mathfrak{D}}(7, 5) = 0.$$

In the case of $r=3$, the first example of relations is obtained from the matrix

$$\mathcal{E}_{15,3} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -6 & -6 & 1 & 6 & 6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -6 & 0 & -6 & 1 & 6 & 6 & 0 & 0 \\ 0 & 0 & 0 & -6 & 0 & 0 & 0 & -5 & 6 & 6 \\ -15 & -14 & 0 & 15 & 0 & 0 & 0 & 15 & 0 & 0 \\ 0 & 0 & 0 & -15 & -14 & 0 & 0 & 0 & 15 & 15 \\ -27 & -42 & 42 & 0 & 0 & 0 & -42 & 0 & 42 & 28 \end{pmatrix}.$$

This has the right annihilator ${}^t(-14,15,6,0,0,36,0,0,0,0)$, which gives

$$-14\zeta_{\mathfrak{D}}(3,3,9)+15\zeta_{\mathfrak{D}}(3,5,7)+6\zeta_{\mathfrak{D}}(3,7,5)+36\zeta_{\mathfrak{D}}(5,5,5)=0.$$

We also give an example for $r=4$: computing the right annihilator of the matrix $\mathcal{E}_{18,4}$, we obtain

$$70\zeta_{\mathfrak{D}}(3,3,3,9)-75\zeta_{\mathfrak{D}}(3,3,5,7)-30\zeta_{\mathfrak{D}}(3,3,7,5)+36\zeta_{\mathfrak{D}}(3,5,5,5)=0.$$

For the proof of Proposition 2.4, we use a result obtained by Brown [3, Section 10]. Set the $|S_{k,r}|\times|S_{k,r}|$ matrix

$$\mathcal{E}^{(r)}_{k,q} = \left(\delta_{(s_1,\ldots,s_{r-q}),(k_1,\ldots,k_{r-q})}\cdot \varepsilon_{\binom{s_{r-q+1},\ldots,s_r}{k_{r-q+1},\ldots,k_r}}\right)_{\substack{(s_1,\ldots,s_r)\in S_{k,r}\\ (k_1,\ldots,k_r)\in S_{k,r}}} \quad (2\le q\le r-1) \qquad (2.12)$$

and define

$$\mathcal{C}_{k,r} = \mathcal{E}^{(r)}_{k,2}\cdot\mathcal{E}^{(r)}_{k,3}\cdots\mathcal{E}^{(r)}_{k,r-1}\cdot\mathcal{E}_{k,r}. \qquad (2.13)$$

(Note that $\mathcal{C}_{k,2}=\mathcal{E}_{k,2}$.)

Proposition 2.5. (Brown [3, Section 10]) *For any right annihilator* $(a_{k_1,\ldots,k_r})_{(k_1,\ldots,k_r)\in S_{k,r}}$ *of the matrix* $\mathcal{C}_{k,r}$*, we have*

$$\sum_{(k_1,\ldots,k_r)\in S_{k,r}} a_{k_1,\ldots,k_r}\zeta_{\mathfrak{D}}(k_1,\ldots,k_r)=0.$$

Proposition 2.4 follows immediately from this and (2.13). We note that, in Brown's original assertion (see [3, Section 10]), he uses an integer $c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ obtained by the "Ihara action" for the definition of the matrix $\mathcal{C}_{k,r}$. Hence we have to check that the integer $c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ corresponds to the $((s_1,\dots,s_r),(k_1,\dots,k_r))$-th entry of our matrix $\mathcal{C}_{k,r}$ for all $(s_1,\dots,s_r),(k_1,\dots,k_r)\in S_{k,r}$. Denote by $\underline{\circ} : \mathbb{Q}[x_1,\dots,x_r]\otimes_{\mathbb{Q}}\mathbb{Q}[x_1,\dots,x_s]\to \mathbb{Q}[x_1,\dots,x_{r+s}]$ the Ihara action computed explicitly by Brown [3, Section 6]. We use the explicit formula

$$\begin{aligned}&f(x_1)\,\underline{\circ}\,g(x_1,\dots,x_{r-1}) = f(x_1)g(x_2,\dots,x_r)\\ &+\sum_{i=1}^{r-1}\big(f(x_{i+1}-x_i)g(x_1,\dots,\hat{x}_{i+1},\dots,x_r)-(-1)^{\deg f}f(x_i-x_{i+1})g(x_1,\dots,\hat{x}_i,\dots,x_r)\big)\end{aligned}$$

to define the integer $c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ as the coefficient of $x_1^{k_1-1}\cdots x_r^{k_r-1}$ in

$$x_1^{s_1-1}\,\underline{\circ}\,(\cdots x_1^{s_{r-2}-1}\,\underline{\circ}\,(x_1^{s_{r-1}-1}\,\underline{\circ}\,x_1^{s_r-1})\cdots) = \sum_{\substack{k_1+\cdots+k_r=s_1+\cdots+s_r\\ k_1,\dots,k_r\ge 1}} c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}} x_1^{k_1-1}\cdots x_r^{k_r-1}. \tag{2.14}$$

Then our task is to prove

$$\Big(c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}\Big)_{\substack{(s_1,\dots,s_r)\in S_{k,r}\\ (k_1,\dots,k_r)\in S_{k,r}}} = \mathcal{C}_{k,r}. \tag{2.15}$$

Note that, for integers $s_i,k_i\ge 1$, it is easily seen that the integer $\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ in (2.1) is equal to the coefficient of $x_1^{k_1-1}\cdots x_r^{k_r-1}$ in $x_1^{s_1-1}\,\underline{\circ}\,(x_1^{s_2-1}\cdots x_{r-1}^{s_r-1})$:

$$x_1^{s_1-1}\,\underline{\circ}\,(x_1^{s_2-1}\cdots x_{r-1}^{s_r-1}) = \sum_{\substack{k_1+\cdots+k_r=s_1+\cdots+s_r\\ k_1,\dots,k_r\ge 1}} \varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}} x_1^{k_1-1}\cdots x_r^{k_r-1}. \tag{2.16}$$

The equality (2.15) is verified by induction on r. From the definition of $c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}$ in (2.14), the equality (2.15) comes from (2.16) when $r=2$. Let

$$\begin{aligned}f(x_1,\dots,x_{r-1}) &= x_1^{s_2-1}\,\underline{\circ}\,(\cdots(x_{r-2}^{s_{r-1}-1}\,\underline{\circ}\,x_{r-1}^{s_r-1})\cdots)\\ &= \sum_{\substack{k_2+\cdots+k_r=s_2+\cdots+s_r\\ k_2,\dots,k_r\ge 1}} c_{\binom{s_2,\dots,s_r}{k_2,\dots,k_r}} x_1^{k_2-1}\cdots x_{r-1}^{k_r-1}.\end{aligned}$$

With (2.16), one computes

$$
\begin{aligned}
x_1^{s_1-1} \,\underline{\circ}\, f(x_1,\dots,x_{r-1}) &= \sum_{t_2+\cdots+t_r=s_2+\cdots+s_r} c_{\binom{s_2,\dots,s_r}{t_2,\dots,t_r}} x_1^{s_1-1} \,\underline{\circ}\, (x_1^{t_2-1}\cdots x_{r-1}^{t_r-1})\\
&= \sum_{t_1+\cdots+t_r=k} \delta_{s_1,t_1} c_{\binom{s_2,\dots,s_r}{t_2,\dots,t_r}} x_1^{t_1-1} \,\underline{\circ}\, (x_1^{t_2-1}\cdots x_{r-1}^{t_r-1})\\
&= \sum_{t_1+\cdots+t_r=k} \delta_{s_1,t_1} c_{\binom{s_2,\dots,s_r}{t_2,\dots,t_r}} \sum_{k_1+\cdots+k_r=k} \varepsilon_{\binom{t_1,\dots,t_r}{k_1,\dots,k_r}} x_1^{k_1-1}\cdots x_r^{k_r-1}\\
&= \sum_{k_1+\cdots+k_r=k} \Big(\sum_{t_1+\cdots+t_r=k} \delta_{s_1,t_1} c_{\binom{s_2,\dots,s_r}{t_2,\dots,t_r}} \varepsilon_{\binom{t_1,\dots,t_r}{k_1,\dots,k_r}} \Big) x_1^{k_1-1}\cdots x_r^{k_r-1},
\end{aligned}
$$

where $k=s_1+\cdots+s_r$. Then, since $x_1^{s_1-1} \,\underline{\circ}\, f(x_1,\dots,x_{r-1}) = \sum c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}} x_1^{k_1-1}\cdots x_r^{k_r-1}$ and, for $(s_1,\dots,s_r),(k_1,\dots,k_r)\in S_{k,r}$, $\delta_{s_1,t_1} c_{\binom{s_2,\dots,s_r}{t_2,\dots,t_r}} \varepsilon_{\binom{t_1,\dots,t_r}{k_1,\dots,k_r}} = 0$ if $(t_1,\dots,t_r)\notin S_{k,r}$, we obtain

$$
c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}} = \sum_{(t_1,\dots,t_r)\in S_{k,r}} \delta_{s_1,t_1} c_{\binom{s_2,\dots,s_r}{t_2,\dots,t_r}} \varepsilon_{\binom{t_1,\dots,t_r}{k_1,\dots,k_r}}.
$$

Combining this and the induction hypothesis

$$
\begin{aligned}
\Big(c_{\binom{s_2,\dots,s_r}{k_2,\dots,k_r}} \Big)_{\substack{(s_2,\dots,s_r)\in S_{k,r-1}\\(k_2,\dots,k_r)\in S_{k,r-1}}} &= \Big(\delta_{(s_2,\dots,s_{r-2}),(k_2,\dots,k_{r-2})} \varepsilon_{\binom{s_{r-1},s_r}{k_{r-1},k_r}} \Big)_{\substack{(s_2,\dots,s_r)\in S_{k,r-1}\\(k_2,\dots,k_r)\in S_{k,r-1}}}\\
&\times \Big(\delta_{(s_2,\dots,s_{r-3}),(k_2,\dots,k_{r-3})} \varepsilon_{\binom{s_{r-2},s_{r-1},s_r}{k_{r-2},k_{r-1},k_r}} \Big)_{\substack{(s_2,\dots,s_r)\in S_{k,r-1}\\(k_2,\dots,k_r)\in S_{k,r-1}}} \cdots \Big(\varepsilon_{\binom{s_2,\dots,s_r}{k_2,\dots,k_r}} \Big)_{\substack{(s_2,\dots,s_r)\in S_{k,r-1}\\(k_2,\dots,k_r)\in S_{k,r-1}}},
\end{aligned}
$$

we obtain the equality (2.15).

Before going to next, we introduce a conjecture on the rank of $\mathcal{C}_{k,r}$. This was given by Brown [3]: the rank of $\mathcal{C}_{k,r}$ is equal to the coefficient of $x^k y^r$ in the power series expansion of (1.1), i.e.

$$
1 + \sum_{k>r>0} \operatorname{rank} \mathcal{C}_{k,r} x^k y^r \overset{?}{=} \frac{1}{1-\mathbb{O}(x)y+\mathbb{S}(x)y^2}. \tag{2.17}
$$

This is called the 'uneven' part of motivic Broadhurst-Kreimer conjecture, and suggests that all linear relations among totally odd MZVs of weight k and depth r arise from the right kernel of the matrix $\mathcal{C}_{k,r}$. In Section 3, we will show that the rank of $\mathcal{C}_{k,4}$ does not exceed the coefficient of $x^k y^4$ in the power series expansion of the right-hand side of (2.17). Theorem 1.2 then follows from

$$\dim \mathcal{Z}_{k,r}^{\mathrm{odd}} \leq \operatorname{rank} \mathcal{C}_{k,r}. \tag{2.18}$$

2.3 Connection with multiple Eisenstein series

The multiple Eisenstein series was first considered by Gangl, Kaneko and Zagier [6, Section 7]. There is an interesting correspondence, observed by Masanobu Kaneko, Stephanie Belcher and others, between the Fourier coefficient of the multiple Eisenstein series and the coefficient obtained from the expansion of the Ihara coaction acting on the motivic MZVs. In this subsection, we present a direct relation.

Throughout this paper, we assume that τ is an element on the upper half-plane.

Definition 2.6. *For $\mathbf{k} = (k_1, \ldots, k_r) \in \mathbb{Z}_{\geq 2}^r$ with $k_r \geq 3$, we define the multiple Eisenstein series $G_{\mathbf{k}}(\tau)$ by*

$$G_{\mathbf{k}}(\tau) = G_{k_1,\ldots,k_r}(\tau) = \frac{1}{(2\pi\sqrt{-1})^{\mathrm{wt}(\mathbf{k})}} \sum_{\substack{0<\lambda_1<\cdots<\lambda_r \\ \lambda_i \in \mathbb{Z}\tau+\mathbb{Z}}} \frac{1}{\lambda_1^{k_1} \cdots \lambda_r^{k_r}}.$$

Here the positivity $m\tau + n > 0$ of a lattice point means either $m > 0$ or $m = 0, n > 0$, and $m\tau + n > m'\tau + n'$ means $(m - m')\tau + (n - n') > 0$.

Since the multiple Eisenstein series $G_{\mathbf{k}}(\tau)$ satisfies $G_{\mathbf{k}}(\tau+1) = G_{\mathbf{k}}(\tau)$, it has the Fourier expansion. A formula of this was given by Henrik Bachman in his master thesis [2].

Proposition 2.7. (Bachmann [2]) *For $\mathbf{k} = (k_1, \ldots, k_r) \in \mathbb{Z}_{\geq 2}^r$ with $k_r \geq 3$ and $k = \mathrm{wt}(\mathbf{k})$, the Fourier expansion of $G_{\mathbf{k}}(\tau)$ can be written in the form*

$$\begin{aligned} G_{k_1,\ldots,k_r}(\tau) &= \widetilde{\zeta}(k_1, \ldots, k_r) + \sum_{s_1+s_2=k} \xi_{s_1}^{(r-1)} g_{s_2}(\tau) + \sum_{s_1+s_2+s_3=k} \xi_{s_1}^{(r-2)} g_{s_2,s_3}(\tau) \\ &+ \sum_{s_1+\cdots+s_4=k} \xi_{s_1}^{(r-3)} g_{s_2,s_3,s_4}(\tau) + \cdots + \sum_{s_1+\cdots+s_{r-1}=k} \xi_{s_1}^{(2)} g_{s_2,\ldots,s_{r-1}}(\tau) \\ &+ \sum_{s_1+\cdots+s_r=k} \xi_{s_1}^{(1)} g_{s_2,\ldots,s_r}(\tau) + g_{k_1,\ldots,k_r}(\tau) \end{aligned}$$

with some $\xi^{(d)}_{s_1} \in \left\langle \widetilde{\zeta}(\mathbf{k}) = \zeta(\mathbf{k})/\bigl(2\pi\sqrt{-1}\bigr)^{\mathrm{wt}(\mathbf{k})} \mid \zeta(\mathbf{k}) \in \mathcal{Z}^{(d)}_{s_1} \right\rangle_{\mathbb{Q}}$, *where*

$$g_{k_1,\ldots,k_r}(\tau) = \sum_{\substack{0<u_1<\cdots<u_r \\ v_1,\ldots,v_r\in\mathbb{Z}_{>0}}} \frac{v_1^{k_1-1}\cdots v_r^{k_r-1}}{(k_1-1)!\cdots(k_r-1)!} q^{u_1v_1+\cdots+u_rv_r} \quad \bigl(q = e^{2\pi\sqrt{-1}\tau}\bigr).$$

We now show a direct relation between the integer $\varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$ and the Fourier expansion of the multiple Eisenstein series. Calculating the coefficient of $\widetilde{\zeta}(s_1)g_{s_2,\ldots,s_r}(\tau)$ in the above Fourier expansion of the multiple Eisenstein series, we can obtain the integer $\varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$ again.

Theorem 2.8. *For integers* $k_r \geq 3$ *and* $k_i \geq 2$ $(1 \leq i \leq r-1)$, *we have*

$$\xi^{(1)}_{s_1} = \varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}} \widetilde{\zeta}(s_1).$$

Proof. The sum of the defining series $G_{k_1,\ldots,k_r}(\tau)$ can be divided into

$$\begin{aligned} \sum_{0<m_1\tau+n_1<\ldots<m_r\tau+n_r} &= \sum_{\substack{0=m_1=\cdots=m_r \\ 0<n_1<\cdots<n_r}} \\ &+ \sum_{\substack{0<m_1=\cdots=m_r \\ n_1<\cdots<n_r}} + \sum_{\substack{0=m_1<m_2=\cdots=m_r \\ n_1>0,n_2<\cdots<n_r}} + \cdots + \sum_{\substack{0=m_1=\cdots m_{r-1}<m_r \\ 0<n_1<\cdots<n_{r-1},n_r\in\mathbb{Z}}} \\ &+ \cdots \\ &+ \sum_{\substack{0<m_1<\cdots<m_{r-1}=m_r \\ n_1,\ldots,n_{r-2}\in\mathbb{Z},n_{r-1}<n_r}} + \cdots + \sum_{\substack{0<m_1<\cdots<m_{r-2}=m_{r-1}<m_r \\ n_1,\ldots,n_{r-3},n_r\in\mathbb{Z},n_{r-2}<n_{r-1}}} + \sum_{\substack{0=m_1<\cdots<m_r \\ n_1>0,n_2\ldots,n_r\in\mathbb{Z}}} \\ &+ \sum_{\substack{0<m_1<\cdots<m_r \\ n_1,\ldots,n_r\in\mathbb{Z}}}. \end{aligned}$$

Set

$$\varPsi_{k_1,\ldots,k_r}(\tau) = \frac{1}{(2\pi\sqrt{-1})^{k_1+\cdots+k_r}} \sum_{n_1<\cdots<n_r} \frac{1}{(\tau+n_1)^{k_1}\cdots(\tau+n_r)^{k_r}}.$$

Then, the forth line in the above decomposition can be computed as

$$\sum_{0<m_1<\cdots<m_{r-1}=m_r} \Psi_{k_1}(m_1\tau)\cdots\Psi_{k_{r-2}}(m_{r-2}\tau)\Psi_{k_{r-1},k_r}(m_r\tau)+\cdots$$
$$+\sum_{0=m_1=m_2<\cdots<m_r} \Psi_{k_1,k_2}(m_1\tau)\Psi_{k_3}(m_3\tau)\cdots\Psi_{k_r}(m_r\tau)+\widetilde{\zeta}(k_1)\sum_{0<m_2<\cdots<m_r}\Psi_{k_2}(m_2\tau)\cdots\Psi_{k_r}(m_r\tau)$$
$$=\sum_{\substack{s_1+\cdots+s_r=k\\ s_1\geq 3,\, s_2,\ldots,s_r\geq 1}} \varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}\widetilde{\zeta}(s_1)g_{s_2,\ldots,s_r}(\tau).$$

Here we used the standard facts that

$$\Psi_{k_i,k_{i+1}}(\tau)=\sum_{\substack{s_1+s_{i+1}=k_i+k_{i+1}\\ s_1\geq 2,\, s_{i+1}\geq 1}}\left((-1)^{k_i}\binom{s_1-1}{k_i-1}+(-1)^{s_1-k_{i+1}}\binom{s_1-1}{k_{i+1}-1}\right)\widetilde{\zeta}(s_1)\Psi_{s_{i+1}}(\tau)$$

and

$$g_{s_1,\ldots,s_r}(\tau)=\sum_{0<m_1<\cdots<m_r}\Psi_{s_1}(m_1\tau)\cdots\Psi_{s_r}(m_r\tau).$$

□

3 Proof of Theorem 1.2

As mentioned in the end of Section 2.2, we compute the rank of $\mathcal{C}_{k,4}$, or equivalently $\dim\ker\mathcal{C}_{k,4}$, to prove Theorem 1.2. Recall

$$\mathcal{E}_{k,3}^{(4)}=\left(\delta_{s_1,k_1}\varepsilon_{\binom{s_2,s_3,s_4}{k_2,k_3,k_4}}\right)_{\substack{(s_1,\ldots,s_4)\in S_{k,4}\\ (k_1,\ldots,k_4)\in S_{k,4}}},\ \mathcal{E}_{k,2}^{(4)}=\left(\delta_{(s_1,s_2),(k_1,k_2)}\varepsilon_{\binom{s_3,s_4}{k_3,k_4}}\right)_{\substack{(s_1,\ldots,s_4)\in S_{k,4}\\ (k_1,\ldots,k_4)\in S_{k,4}}}.$$

The matrix $\mathcal{C}_{k,4}$ is defined by $\mathcal{C}_{k,4}=\mathcal{E}_{k,2}^{(4)}\cdot\mathcal{E}_{k,3}^{(4)}\cdot\mathcal{E}_{k,4}$.

3.1 Shuffle algebra

Let $\mathfrak{V}$ be a bigraded vector space over $\mathbb{Q}$ spanned by all words in noncommutative symbols $\{z_{2i+1}\mid i\geq 1\}$:

$$\mathfrak{V}=\mathbb{Q}\langle z_3,z_5,z_7,\ldots\rangle=\mathbb{Q}\oplus\bigoplus_{k>r>0}\mathfrak{V}_{k,r},$$

where $\mathfrak{V}_{k,r}$ is the $\mathbb{Q}$-vector space spanned by the set $\{z_{k_1}\cdots z_{k_r} \mid (k_1,\ldots,k_r)\in S_{k,r}\}$, and the empty word is regarded as 1. Then the vector space $\mathfrak{V}$ becomes a bigraded commutative algebra over $\mathbb{Q}$ with respect to the shuffle product ш:

$$z_{k_1}\cdots z_{k_r} \mathbin{ш} z_{k_{r+1}}\cdots z_{k_{r+s}} = \sum_{\substack{\sigma\in\mathfrak{S}_{r+s}\\ \sigma(1)<\cdots<\sigma(r)\\ \sigma(r+1)<\cdots<\sigma(r+s)}} z_{k_{\sigma^{-1}(1)}}\cdots z_{k_{\sigma^{-1}(r+s)}}. \tag{3.1}$$

The important fact is that the algebra $\mathfrak{V}$ is isomorphic to the polynomial algebra in the Lyndon words (see [12]). Therefore, for example, we see that the set of monomials in the Lyndon words $\{z_{k_1}z_{k_2}, z_{s_1} \mathbin{ш} z_{s_2} \mid (k_1,k_2),(s_1,s_2)\in S_{k,2}, k_1<k_2, s_1\le s_2\}$ is a basis of $\mathfrak{V}_{k,2}$.

Proposition 3.1. *For any odd integer $p\ge 3$, the set $\{z_p \mathbin{ш} z_{k_1}z_{k_2}z_{k_3} \mid (k_1,k_2,k_3)\in S_{k,3}\}$ is linearly independent over $\mathbb{Q}$.*

Proof. For convenience, we put $d=\dim\mathfrak{V}_{k,3}=|S_{k,3}|$ and $\{z_{k_1}z_{k_2}z_{k_3} \mid (k_1,k_2,k_3)\in S_{k,3}\} = \{v_i\}_{i=1}^d$. Let $\{v_i'\}_{i=1}^d$ be the basis of $\mathfrak{V}_{k,3}$ consisting of monomials in the Lyndon words (with respect to the shuffle product ш). Then, we find that the set $\{z_p \mathbin{ш} v_i' \mid 1\le i\le d\}$ is linearly independent. We write $v_i=\sum_{j=1}^d a_{i,j}v_j'$ and set the $d\times d$ matrix $A=(a_{i,j})$. Assuming $\sum_{i=1}^d p_i\big(z_p \mathbin{ш} v_i\big)=0$ for $p_i\in\mathbb{Q}$, we have

$$\sum_{j=1}^d\sum_{i=1}^d p_i a_{i,j}\big(z_p \mathbin{ш} v_j'\big)=0,$$

which implies $(p_1,\ldots,p_d)\cdot A=0$. Since the matrix A is invertible, we have $p_i=0$ for all i, which completes the proof. □

Proposition 3.2. *(i) For odd integers $k_1,k_2\ge 3$ $(k_1\ne k_2)$, we denote by $\{v_1,\ldots,v_g\}$ (resp. $\{w_1,\ldots,w_h\}$) a basis of $\mathfrak{V}_{k_1,2}$ (resp. $\mathfrak{V}_{k_2,2}$). Then the set $\{v_i \mathbin{ш} w_j \mid 1\le i\le g,\ 1\le j\le h\}$ is linearly independent over $\mathbb{Q}$.*
(ii) For an odd integer $k\ge 3$, denote by $\{v_1,\ldots,v_g\}$ a basis of $\mathfrak{V}_{k,2}$. Then the set $\{v_i \mathbin{ш} v_j \mid 1\le i\le j\le g\}$ is linearly independent over $\mathbb{Q}$.

Proof. For (i), let $\{v_i'\}_{i=1}^g$ (resp. $\{w_i'\}_{i=1}^h$) be the basis of $\mathfrak{V}_{k_1,2}$ (resp. $\mathfrak{V}_{k_2,2}$) consisting of monomials in the Lyndon words. We write $v_i=\sum a_{i,j}v_j'$ (resp. $w_i=\sum b_{i,j}w_j'$), and set the $g\times g$ (resp. $h\times h$) matrix $A=(a_{i,j})$ (resp. $B=(b_{i,j})$). Assuming

$\sum p_{i_1,i_2}(v_{i_1} \sqcup\!\sqcup\, w_{i_2}) = 0$ for $p_{i_1,i_2} \in \mathbb{Q}$, we compute

$$\begin{aligned}
0 &= \sum_{\substack{1 \le i_1 \le g \\ 1 \le i_2 \le h}} p_{i_1,i_2}(v_{i_1} \sqcup\!\sqcup\, w_{i_2}) \\
&= \sum_{\substack{1 \le i_1 \le g \\ 1 \le i_2 \le h}} p_{i_1,i_2}\Big(\sum_{1 \le j_1 \le g} a_{i_1,j_1} v'_{j_1}\Big) \sqcup\!\sqcup\, \Big(\sum_{1 \le j_2 \le h} b_{i_2,j_2} w'_{j_2}\Big) \\
&= \sum_{\substack{1 \le j_1 \le g \\ 1 \le j_2 \le h}} \Big(\sum_{\substack{1 \le i_1 \le g \\ 1 \le i_2 \le h}} p_{i_1,i_2} a_{i_1,j_1} b_{i_2,j_2}\Big) v'_{j_1} \sqcup\!\sqcup\, w'_{j_2}.
\end{aligned}$$

Since the set $\{v'_{j_1} \sqcup\!\sqcup\, w'_{j_2} \mid 1 \le j_1 \le g, 1 \le j_2 \le h\}$ is linearly independent, for each j_1, j_2 ($1 \le j_1 \le g$, $1 \le j_2 \le h$) we obtain

$$\sum_{1 \le i_2 \le h} q_{i_2}^{(j_1)} b_{i_2,j_2} = 0,$$

where $q_{i_2}^{(j_1)} = \sum_{1 \le i_1 \le g} p_{i_1,i_2} a_{i_1,j_1}$. This shows that for any j_1 ($1 \le j_1 \le g$), we have $(q_1^{(j_1)}, \dots, q_h^{(j_1)}) \cdot B = 0$, and hence $(q_1^{(j_1)}, \dots, q_h^{(j_1)}) = 0$, because the matrix B is invertible. Therefore for each i_2, j_1 ($1 \le i_2 \le h$, $1 \le j_1 \le g$) we have

$$\sum_{1 \le i_1 \le g} p_{i_1,i_2} a_{i_1,j_1} = 0,$$

which implies $(p_{1,i_2}, \dots, p_{g,i_2}) \cdot A = 0$. This gives $p_{i_1,i_2} = 0$ for all i_1, i_2.
(ii) Similarly, we assume

$$\begin{aligned}
0 &= \sum_{1 \le i_1, i_2 \le g} p_{i_1,i_2}(v_i \sqcup\!\sqcup\, v_j) \\
&= \sum_{1 \le j_1, j_2 \le g} \Big(\sum_{1 \le i_1, i_2 \le g} p_{i_1,i_2} a_{i_1,j_1} a_{i_2,j_2}\Big) v'_{j_1} \sqcup\!\sqcup\, v'_{j_2}
\end{aligned}$$

for $p_{i_1,i_2} \in \mathbb{Q}$ with $p_{i_1,i_2} = 0$ if $i_1 > i_2$. Since the set $\{v'_i \sqcup\!\sqcup\, v'_j \mid 1 \le i_1 \le i_2 \le g\}$ is linearly independent, for any j_1, j_2 ($1 \le j_1, j_2 \le g$), we find

$$\begin{aligned}
0 &= \sum_{1 \le i_1, i_2 \le g} p_{i_1,i_2} a_{i_1,j_1} a_{i_2,j_2} + \sum_{1 \le i_1, i_2 \le g} p_{i_1,i_2} a_{i_1,j_2} a_{i_2,j_1} \\
&= \sum_{1 \le i_1, i_2 \le g} (p_{i_1,i_2} + p_{i_2,i_1}) a_{i_1,j_1} a_{i_2,j_2}.
\end{aligned}$$

Putting $P_{i_1,i_2} = p_{i_1,i_2} + p_{i_2,i_1}$, we can prove $P_{i_1,i_2} = 0$ for all i_1, i_2 $(1 \leq i_1, i_2 \leq g)$ in much the same way as in the proof of (i). Since

$$P_{i_1,i_2} = \begin{cases} p_{i_1,i_2} & i_1 < i_2 \\ 2p_{i_1,i_1} & i_1 = i_2 \\ p_{i_2,i_1} & i_1 > i_2 \end{cases},$$

we have $p_{i_1,i_2} = 0$ for all i_1, i_2. □

Corollary 3.3. *Let V_1 and V_2 be subspaces of $V_{k_1,2}$ and $V_{k_2,2}$ respectively. We define the subspace $S(V_1, V_2)$ of $V_{k_1+k_2,4}$ by*

$$S(V_1, V_2) = \left\langle w_1 ш w_2 \mid w_1 \in V_1, w_2 \in V_2 \right\rangle_{\mathbb{Q}}.$$

Then, if $V_1 \cap V_2 = 0$, we have

$$\dim S(V_1, V_2) = \dim V_1 \times \dim V_2,$$

and if $V_1 \supset V_2$, we obtain

$$\dim S(V_1, V_2) = \dim V_1 \times \dim V_2 - \sharp\{(i,j) \mid 1 \leq i < j \leq \dim V_2\}.$$

Proof. This is a direct consequence of Proposition 3.2. □

3.2 Key identities

We start with a discussion of $\ker {}^t\mathcal{E}_{k,q}^{(r)}$. By definition (2.12), for $q \in \{2, \ldots, r-1\}$ the matrix $\mathcal{E}_{k,q}^{(r)}$ can be expressed as the direct sum

$$\begin{aligned} \mathcal{E}_{k,q}^{(r)} &= \bigoplus_{\substack{1<p<k \\ (p_1,\ldots,p_{r-q}) \in S_{p,r-q}}} \mathcal{E}_{k-p,q} \\ &= diag(\underbrace{\mathcal{E}_{3q,q}, \ldots, \mathcal{E}_{3q,q}}_{|S_{k-3q,r-q}|}, \underbrace{\mathcal{E}_{3q+2,q}, \ldots \mathcal{E}_{3q+2,q}}_{|S_{k-3q-2,r-q}|}, \ldots, \mathcal{E}_{k-3(r-q),q}). \end{aligned}$$

We therefore have

$$\ker {}^t\mathcal{E}_{k,q}^{(r)} = \bigoplus_{\substack{1<p<k \\ (p_1,\dots,p_{r-q})\in S_{p,r-q}}} \langle \iota_{p_1,\dots,p_{r-q}}(v) \mid v \in \ker {}^t\mathcal{E}_{k-p,q}\rangle_{\mathbb{Q}}, \tag{3.2}$$

where the injective linear map $\iota_{p_1,\dots,p_{r-q}}$ is defined by

$$\begin{aligned} \iota_{p_1,\dots,p_{r-q}} : \mathcal{V}_{k-p,q} &\longrightarrow \mathcal{V}_{k,r}, \\ (a_{k_1,\dots,k_q})_{(k_1,\dots,k_q)\in S_{k-p,q}} &\longmapsto \big(\delta_{(p_1,\dots,p_{r-q}),(k_1,\dots,k_{r-q})} \cdot a_{k_{r-q+1},\dots,k_r}\big)_{(k_1,\dots,k_r)\in S_{k,r}}. \end{aligned}$$

The key identities in the proof of Theorem 1.2 are concerning the following two linear maps: for an odd integer $p \geq 3$, set

$$\begin{aligned} \Theta_p : \mathcal{V}_{k-p,3} &\longrightarrow \mathcal{V}_{k,4}, \\ (a_{k_1,k_2,k_3})_{(k_1,k_2,k_3)\in S_{k-p,3}} &\longmapsto \Big(\sum_{\substack{\sigma\in\mathfrak{S}_4 \\ \sigma(2)<\sigma(3)<\sigma(4)}} \delta_{p,k_{\sigma(1)}} \cdot a_{k_{\sigma(2)},k_{\sigma(3)},k_{\sigma(4)}}\Big)_{(k_1,k_2,k_3,k_4)\in S_{k,4}}, \end{aligned} \tag{3.3}$$

and, for an even integer $p \geq 6$ and $(p_1,p_2) \in S_{p,2}$, set

$$\begin{aligned} \Theta_{p_1,p_2} : \mathcal{V}_{k-p,2} &\longrightarrow \mathcal{V}_{k,4}, \\ (a_{k_1,k_2})_{(k_1,k_2)\in S_{k-p,2}} &\longmapsto \Big(\sum_{\substack{\sigma\in\mathfrak{S}_4 \\ \sigma(1)<\sigma(2) \\ \sigma(3)<\sigma(4)}} \delta_{(p_1,p_2),(k_{\sigma(1)},k_{\sigma(2)})} \cdot a_{k_{\sigma(3)},k_{\sigma(4)}}\Big)_{(k_1,k_2,k_3,k_4)\in S_{k,4}}. \end{aligned} \tag{3.4}$$

We note that using an isomorphism $\pi : \mathcal{V}_{k,r} \to \mathfrak{V}_{k,r}$ given by $(a_{s_1,\dots,s_r})_{(s_1,\dots,s_r)\in S_{k,r}} \mapsto \sum_{(s_1,\dots,s_r)\in S_{k,r}} a_{s_1,\dots,s_r} z_{s_1}\cdots z_{s_r}$, one has $\pi\big(\Theta_p(v)\big) = z_p ш \sum_{(s_1,s_2,s_3)\in S_{k,3}} a_{s_1,s_2,s_3} z_{s_1}z_{s_2}z_{s_3}$ for $v = (a_{s_1,s_2,s_3})_{(s_1,s_2,s_3)\in S_{k,3}} \in \mathcal{V}_{k,3}$, and $\pi\big(\Theta_{p_1,p_2}(v)\big) = z_{p_1}z_{p_2} ш \sum_{(s_1,s_2)\in S_{k,2}} a_{s_1,s_2} z_{s_1}z_{s_2}$ for $v = (a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}} \in \mathcal{V}_{k,2}$, because of (3.1). Therefore, by Propositions 3.1 and 3.2, we find that the maps Θ_p and Θ_{p_1,p_2} are injective.

Lemma 3.4. *(i) For each odd integer $p \geq 3$ and $v \in \ker {}^t\mathcal{E}_{k-p,3}$, we have*

$${}^t\mathcal{E}_{k,4}\big(\Theta_p(v)\big) = \iota_p(v) \in \ker {}^t\mathcal{E}_{k,3}^{(4)}. \tag{3.5}$$

(ii) For each even integer $p \geq 6$, $(p_1,p_2) \in S_{p,2}$ and $v \in \ker {}^t\mathcal{E}_{k-p,2}$, we have

$${}^t\mathcal{E}_{k,3}^{(4)}\big({}^t\mathcal{E}_{k,4}\big(\Theta_{p_1,p_2}(v)\big)\big) = \sum_{(t_1,t_2)\in S_{p,2}} \varepsilon_{\binom{t_1,t_2}{p_1,p_2}} \iota_{t_1,t_2}(v) \in \ker {}^t\mathcal{E}_{k,2}^{(4)}. \tag{3.6}$$

Proof. These are shown by direct calculations. For (i), let $v = (a_{k_1,k_2,k_3})_{(k_1,k_2,k_3)\in S_{k-p,3}}$. For $(k_1,\ldots,k_4) \in S_{k,4}$ we denote by $b^{(p)}_{k_1,\ldots,k_4}$ the $(k_1,\ldots,k_4)$-th entry of the vector $\Theta_p(v)$, so that $b^{(p)}_{k_1,\ldots,k_4} = \delta_{p,k_1} a_{k_2,k_3,k_4} + \delta_{p,k_2} a_{k_1,k_3,k_4} + \delta_{p,k_3} a_{k_1,k_2,k_4} + \delta_{p,k_4} a_{k_1,k_2,k_3}$. Then the $(s_1,\ldots,s_4)$-th entry of the vector ${}^t\mathcal{E}_{k,4}(\Theta_p(v))$ can be computed as follows:

$$
\begin{aligned}
&b^{(p)}_{s_1,\ldots,s_4} + \sum_{(k_1,\ldots,k_4)\in S_{k,4}} b^{(p)}_{k_1,\ldots,k_4}\big(\delta_{(s_3,s_4),(k_3,k_4)} C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_4),(k_1,k_4)} C^{s_1}_{k_2,k_3} + \delta_{(s_2,s_3),(k_1,k_2)} C^{s_1}_{k_3,k_4}\big) \\
&= \delta_{p,s_1} a_{s_2,s_3,s_4} + \delta_{p,s_2} a_{s_1,s_3,s_4} + \delta_{p,s_3} a_{s_1,s_2,s_4} + \delta_{p,s_4} a_{s_1,s_2,s_3} \\
&+ \sum_{(k_2,k_3,k_4)\in S_{k-p,3}} a_{k_2,k_3,k_4}\big(\delta_{(s_3,s_4),(k_3,k_4)} C^{s_1}_{p,k_2} + \delta_{(s_2,s_4),(p,k_4)} C^{s_1}_{k_2,k_3} + \delta_{(s_2,s_3),(p,k_2)} C^{s_1}_{k_3,k_4}\big) \\
&+ \sum_{(k_1,k_3,k_4)\in S_{k-p,3}} a_{k_1,k_3,k_4}\big(\delta_{(s_3,s_4),(k_3,k_4)} C^{s_1}_{k_1,p} + \delta_{(s_2,s_4),(k_1,k_4)} C^{s_1}_{p,k_3} + \delta_{(s_2,s_3),(k_1,p)} C^{s_1}_{k_3,k_4}\big) \\
&+ \sum_{(k_1,k_2,k_4)\in S_{k-p,3}} a_{k_1,k_2,k_4}\big(\delta_{(s_3,s_4),(p,k_4)} C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_4),(k_1,k_4)} C^{s_1}_{k_2,p} + \delta_{(s_2,s_3),(k_1,k_2)} C^{s_1}_{p,k_4}\big) \\
&+ \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{(s_3,s_4),(k_3,p)} C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_4),(k_1,p)} C^{s_1}_{k_2,k_3} + \delta_{(s_2,s_3),(k_1,k_2)} C^{s_1}_{k_3,p}\big) \\
&= \delta_{p,s_1} a_{s_2,s_3,s_4} + \delta_{p,s_2} a_{s_1,s_3,s_4} + \delta_{p,s_3} a_{s_1,s_2,s_4} + \delta_{p,s_4} a_{s_1,s_2,s_3} \\
&+ \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{(s_3,s_4),(k_2,k_3)} C^{s_1}_{p,k_1} + \delta_{(s_2,s_4),(p,k_3)} C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_3),(p,k_1)} C^{s_1}_{k_2,k_3}\big) \\
&+ \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{(s_3,s_4),(k_2,k_3)} C^{s_1}_{k_1,p} + \delta_{(s_2,s_4),(k_1,k_3)} C^{s_1}_{p,k_2} + \delta_{(s_2,s_3),(k_1,p)} C^{s_1}_{k_2,k_3}\big) \\
&+ \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{(s_3,s_4),(p,k_3)} C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_4),(k_1,k_3)} C^{s_1}_{k_2,p} + \delta_{(s_2,s_3),(k_1,k_2)} C^{s_1}_{p,k_3}\big) \\
&+ \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{(s_3,s_4),(k_3,p)} C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_4),(k_1,p)} C^{s_1}_{k_2,k_3} + \delta_{(s_2,s_3),(k_1,k_2)} C^{s_1}_{k_3,p}\big) \\
&= \delta_{p,s_1} a_{s_2,s_3,s_4} + \delta_{p,s_2} a_{s_1,s_3,s_4} + \delta_{p,s_3} a_{s_1,s_2,s_4} + \delta_{p,s_4} a_{s_1,s_2,s_3} \\
&+ \delta_{p,s_2} \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{s_4,k_3} C^{s_1}_{k_1,k_2} + \delta_{s_3,k_1} C^{s_1}_{k_2,k_3}\big) \\
&+ \delta_{p,s_3} \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{s_2,k_1} C^{s_1}_{k_2,k_3} + \delta_{s_4,k_3} C^{s_1}_{k_1,k_2}\big) \\
&+ \delta_{p,s_4} \sum_{(k_1,k_2,k_3)\in S_{k-p,3}} a_{k_1,k_2,k_3}\big(\delta_{s_3,k_3} C^{s_1}_{k_1,k_2} + \delta_{s_2,k_1} C^{s_1}_{k_2,k_3}\big) \\
&= \delta_{p,s_1} a_{s_2,s_3,s_4},
\end{aligned}
$$

where for the third equality we used $C^{s_1}_{k_i,k_j} + C^{s_1}_{k_j,k_i} = 0$ and for the last we used the relation ${}^t\mathcal{E}_{k-p,3}(v) = 0$. This gives (3.5). For (ii), we denote $v = (a_{k_1,k_2})_{(k_1,k_2)\in S_{k-p,2}}$ and $\Theta_{p_1,p_2}(v) = (b^{(p_1,p_2)}_{k_1,\ldots,k_4})_{(k_1,\ldots,k_4)\in S_{k,4}}$ defined in (3.4):

$$\begin{aligned}b^{(p_1,p_2)}_{k_1,\ldots,k_4} &= \delta_{(p_1,p_2),(k_1,k_2)}a_{k_3,k_4} + \delta_{(p_1,p_2),(k_1,k_3)}a_{k_2,k_4} + \delta_{(p_1,p_2),(k_1,k_4)}a_{k_2,k_3}\\ &\quad + \delta_{(p_1,p_2),(k_2,k_3)}a_{k_1,k_4} + \delta_{(p_1,p_2),(k_2,k_4)}a_{k_1,k_3} + \delta_{(p_1,p_2),(k_3,k_4)}a_{k_1,k_2}.\end{aligned}$$

A similar computation shows that the $(s_1,\ldots,s_4)$-th entry of the vector ${}^t\mathcal{E}_{k,4}\big(\Theta_{p_1,p_2}(v)\big)$ can be reduced to

$$\begin{aligned}&b^{(p_1,p_2)}_{s_1,\ldots,s_4} + \sum_{(k_1,\ldots,k_4)\in S_{k,4}} b^{(p_1,p_2)}_{k_1,\ldots,k_4}\big(\delta_{(s_3,s_4),(k_3,k_4)}C^{s_1}_{k_1,k_2} + \delta_{(s_2,s_4),(k_1,k_4)}C^{s_1}_{k_2,k_3} + \delta_{(s_2,s_3),(k_1,k_2)}C^{s_1}_{k_3,k_4}\big)\\ &= C^{s_1}_{p_1,p_2}(a_{s_3,s_4} + a_{s_2,s_4} + a_{s_2,s_3}) + \delta_{(p_1,p_2),(s_1,s_2)}a_{s_3,s_4} + \delta_{(p_1,p_2),(s_1,s_3)}a_{s_2,s_4} + \delta_{(p_1,p_2),(s_2,s_3)}a_{s_2,s_3}.\end{aligned}$$

(Note $a_{s_1,s_2} = 0$ whenever $s_1 + s_2 \neq k - p$.) We denote by $\mathbf{b}^{(p_1,p_2)}_{s_1,\ldots,s_4}$ the right-hand side of the above. With the relation ${}^t\mathcal{E}_{k-p,2}(v) = 0$, we find that the $(s_1,\ldots,s_4)$-th entry of the vector ${}^t\mathcal{E}^{(4)}_{k,3}\big((\mathbf{b}^{(p_1,p_2)}_{k_1,\ldots,k_4})_{(k_1,\ldots,k_4)\in S_{k,4}}\big)$ can be computed as follows:

$$\begin{aligned}&\mathbf{b}^{(p_1,p_2)}_{s_1,\ldots,s_4} + \sum_{(k_1,\ldots,k_4)\in S_{k,4}} \mathbf{b}^{(p_1,p_2)}_{k_1,\ldots,k_4}\big(\delta_{(s_1,s_4),(k_1,k_4)}C^{s_2}_{k_2,k_3} + \delta_{(s_1,s_3),(k_1,k_2)}C^{s_2}_{k_3,k_4}\big)\\ &= \mathbf{b}^{(p_1,p_2)}_{s_1,\ldots,s_4}\\ &+ \sum_{(k_1,\ldots,k_4)\in S_{k,4}} \delta_{(s_1,s_4),(k_1,k_4)}C^{s_2}_{k_2,k_3}\big(\delta_{(p_1,p_2),(k_1,k_2)}a_{k_3,k_4} + \delta_{(p_1,p_2),(k_1,k_3)}a_{k_2,k_4}\\ &+ \delta_{(p_1,p_2),(k_1,k_4)}a_{k_2,k_3} + C^{k_1}_{p_1,p_2}(a_{k_3,k_4} + a_{k_2,k_4} + a_{k_2,k_3})\big)\\ &+ \sum_{(k_1,\ldots,k_4)\in S_{k,4}} \delta_{(s_1,s_3),(k_1,k_2)}C^{s_2}_{k_3,k_4}\big(\delta_{(p_1,p_2),(k_1,k_2)}a_{k_3,k_4} + \delta_{(p_1,p_2),(k_1,k_3)}a_{k_2,k_4}\\ &+ \delta_{(p_1,p_2),(k_1,k_4)}a_{k_2,k_3} + C^{k_1}_{p_1,p_2}(a_{k_3,k_4} + a_{k_2,k_4} + a_{k_2,k_3})\big)\\ &= C^{s_1}_{p_1,p_2}(a_{s_3,s_4} + a_{s_2,s_4} + a_{s_2,s_3}) + \delta_{(p_1,p_2),(s_1,s_2)}a_{s_3,s_4} + \delta_{(p_1,p_2),(s_1,s_3)}a_{s_2,s_4} + \delta_{(p_1,p_2),(s_2,s_3)}a_{s_2,s_3}\\ &+ \sum_{(k_1,\ldots,k_4)\in S_{k,4}} \big(\delta_{(p_1,p_2),(k_1,k_4)}\delta_{(s_1,s_4),(k_1,k_4)}C^{s_2}_{k_2,k_3}a_{k_2,k_3} + \delta_{(p_1,p_2),(k_1,k_2)}\delta_{(s_1,s_3),(k_1,k_2)}C^{s_2}_{k_3,k_4}a_{k_3,k_4}\big)\\ &+ C^{s_1}_{p_1,p_2}\sum_{(k_1,\ldots,k_4)\in S_{k,4}} \big(\delta_{(s_1,s_4),(k_1,k_4)}C^{s_2}_{k_2,k_3}a_{k_2,k_3} + \delta_{(s_1,s_3),(k_1,k_2)}C^{s_2}_{k_3,k_4}a_{k_3,k_4}\big)\\ &= \delta_{(p_1,p_2),(s_1,s_2)}a_{s_3,s_4} + C^{s_1}_{p_1,p_2}a_{s_3,s_4} = \varepsilon_{\binom{s_1,s_2}{p_1,p_2}}a_{s_3,s_4}.\end{aligned}$$

Therefore we have

$$ {}^t\mathcal{E}^{(4)}_{k,3}\big({}^t\mathcal{E}_{k,4}\big(\Theta_{p_1,p_2}(v)\big)\big) = \sum_{(t_1,t_2)\in S_{p,2}} \varepsilon_{\binom{t_1,t_2}{p_1,p_2}} \iota_{t_1,t_2}(v), $$

which is annihilate by ${}^t\mathcal{E}^{(4)}_{k,2}$ because ${}^t\mathcal{E}_{k-p,2}(v)=0$. This gives the assertion (3.6). □

Corollary 3.5. *(i) For $v_p \in \ker {}^t\mathcal{E}_{k-p,3}$ and $a_p \in \mathbb{Q}$, let $v = \sum_{1<p<k} a_p \Theta_p(v_p)$. Then ${}^t\mathcal{E}_{k,4}(v)=0$ if and only if $v=0$.*
(ii) For $v_p \in \ker {}^t\mathcal{E}_{k-p,2}$ and $a^{(p)}_{p_1,p_2} \in \mathbb{Q}$, let $v = \sum_{1<p<k} \sum_{(p_1,p_2)\in S_{p,2}} a^{(p)}_{p_1,p_2} \Theta_{p_1,p_2}(v_p)$. Then ${}^t\mathcal{E}^{(4)}_{k,3}\big({}^t\mathcal{E}_{k,4}(v)\big)=0$ if and only if $(a^{(p)}_{p_1,p_2})_{(p_1,p_2)\in S_{p,2}} \in \ker {}^t\mathcal{E}_{p,2}$ for all p.

Proof. For (i), applying ${}^t\mathcal{E}_{k,4}$ to v, we obtain the assertion from (3.2) and (3.5). For (ii), from (3.6) we have

$$ {}^t\mathcal{E}^{(4)}_{k,3}\big({}^t\mathcal{E}_{k,4}(v)\big) = \sum_{1<p<k} \sum_{(t_1,t_2)\in S_{p,2}} \Bigg(\sum_{(p_1,p_2)\in S_{p,2}} a^{(p)}_{p_1,p_2} \varepsilon_{\binom{t_1,t_2}{p_1,p_2}} \Bigg) \iota_{t_1,t_2}(v_p) \in \ker {}^t\mathcal{E}^{(4)}_{k,2}. $$

By (3.2) the above sum is zero if and only if each coefficients of $\iota_{t_1,t_2}(v_p)$ is zero, i.e. $(a^{(p)}_{p_1,p_2})_{(p_1,p_2)\in S_{p,2}} \in \ker {}^t\mathcal{E}_{p,2}$ for all p. □

3.3 Proof of Theorem 1.2

Note that from (3.2) and Corollary 3.5, for all p $(1<p<k)$ the subspaces $\langle \Theta_p(v) \mid v \in \ker {}^t\mathcal{E}_{k-p,3} \rangle_{\mathbb{Q}}$ of $\mathcal{V}_{k,4}$ only intersect at the zero vector. We set

$$ \mathcal{G}^{(1)}_k = \bigoplus_{1<p<k} \langle \Theta_p(v) \mid v \in \ker {}^t\mathcal{E}_{k-p,3} \rangle_{\mathbb{Q}}. $$

Since the map Θ_p is injective, we obtain $\dim \mathcal{G}^{(1)}_k = \sum_{1<p<k} |S_{p,1}| \cdot \dim \ker {}^t\mathcal{E}_{k-p,3}$. Let

$$ \mathcal{G}^{(2)}_{k,p} = \Bigg\{ \sum_{(p_1,p_2)\in S_{p,2}} a_{p_1,p_2} \Theta_{p_1,p_2}(v) \;\Bigg|\; (a_{p_1,p_2})_{(p_1,p_2)\in S_{p,2}} \in \mathcal{V}_{p,2},\ v \in \ker {}^t\mathcal{E}_{k-p,2} \Bigg\}. $$

Since we find $\pi\big(\mathcal{G}^{(2)}_{k,p}\big) = \langle v ш w \mid v \in \mathfrak{V}_{p,2},\ w \in \pi\big(\ker {}^t\mathcal{E}_{k-p,2}\big) \rangle_{\mathbb{Q}}$, from Corollary 3.3 we obtain

$$ \dim \mathcal{G}^{(2)}_{k,p} = |S_{p,2}| \cdot \dim \ker {}^t\mathcal{E}_{k-p,2} - \delta_{p,k/2} R_p, $$

where $R_p = \sharp\{(i,j) \mid 1 \le i < j \le \dim\ker{}^t\mathcal{E}_{k-p,2}\}$. Note that by Corollary 3.5 (ii) the spaces $\mathcal{G}^{(2)}_{k,p}$ $(1 < p < k)$ only intersect at the zero vector. We put

$$\mathcal{G}^{(2)}_k = \bigoplus_{1<p<k} \mathcal{G}^{(2)}_{k,p}.$$

Corollary 3.5 (i) implies that $\ker{}^t\mathcal{E}_{k,4} \cap \mathcal{G}^{(1)}_k = 0$. Then by Lemma 3.4, we have

$$\ker{}^t\mathcal{C}_{k,4} \supset \big(\ker{}^t\mathcal{E}_{k,4} \oplus \mathcal{G}^{(1)}_k\big) + \mathcal{G}^{(2)}_k.$$

To compute $\dim\ker{}^t\mathcal{C}_{k,4}$, we discuss the intersection of the right-hand side of the above spaces. Since we have $\dim\mathcal{G}^{(1)}_k = \dim\ker{}^t\mathcal{E}^{(4)}_{k,3}$, from Corollary 3.5 (i) we find that the map ${}^t\mathcal{E}_{k,4} : \mathcal{G}^{(1)}_k \to \ker{}^t\mathcal{E}^{(4)}_{k,3}$ is an isomorphism. This shows that for any $v \in \ker{}^t(\mathcal{E}^{(4)}_{k,3} \cdot \mathcal{E}_{k,4})$ we have ${}^t\mathcal{E}_{k,4}(v) \in \ker{}^t\mathcal{E}^{(4)}_{k,3} = {}^t\mathcal{E}_{k,4}\big(\mathcal{G}^{(1)}_k\big)$. Then there exists $v' \in \mathcal{G}^{(1)}_k$ such that $v - v' \in \ker{}^t\mathcal{E}_{k,4}$, which implies $v \in \ker{}^t\mathcal{E}_{k,4} \oplus \mathcal{G}^{(1)}_k$. We therefore have $\ker{}^t(\mathcal{E}^{(4)}_{k,3} \cdot \mathcal{E}_{k,4}) = \ker{}^t\mathcal{E}_{k,4} \oplus \mathcal{G}^{(1)}_k$. From Corollary 3.5 (ii), the intersection of the spaces $\ker{}^t(\mathcal{E}^{(4)}_{k,3} \cdot \mathcal{E}_{k,4})$ and $\mathcal{G}^{(2)}_k$ coincides with the space

$$\bigoplus_{1<p<k} \langle \sum_{(p_1,p_2)\in S_{p,2}} a^{(p)}_{p_1,p_2} \Theta_{p_1,p_2}(v_p) \mid v_p \in \ker{}^t\mathcal{E}_{k-p,2},\ (a^{(p)}_{p_1,p_2})_{(p_1,p_2)\in S_{p,2}} \in \ker{}^t\mathcal{E}_{p,2}\rangle_{\mathbb{Q}},$$

and, by Corollary 3.3, its dimension is given by $\sum_{1<p<k}\big(\dim\ker{}^t\mathcal{E}_{p,2} \cdot \dim\ker{}^t\mathcal{E}_{k-p,2} - \delta_{p,k/2}R_p\big)$. Then we have

$$\begin{aligned}
&\dim\ker{}^t\mathcal{C}_{k,4} \ge \dim\ker{}^t\mathcal{E}_{k,4} + \sum_{1<p<k} |S_{p,1}| \cdot \dim\ker{}^t\mathcal{E}_{k-p,3} \\
&+ \sum_{1<p<k} \big(|S_{p,2}| \cdot \dim\ker{}^t\mathcal{E}_{k-p,2} - \delta_{p,k/2}R_p\big) - \dim(\ker{}^t(\mathcal{E}^{(4)}_{k,3} \cdot \mathcal{E}_{k,4}) \cap \mathcal{G}^{(2)}_k) \\
&= \dim\ker{}^t\mathcal{E}_{k,4} + \sum_{1<p<k} |S_{p,1}| \cdot \dim\ker{}^t\mathcal{E}_{k-p,3} + \sum_{1<p<k} (|S_{p,2}| - \dim\ker{}^t\mathcal{E}_{p,2}) \cdot \dim\ker{}^t\mathcal{E}_{k-p,2}.
\end{aligned}$$

This gives

$$\sum_{k>0} \operatorname{rank} \mathcal{C}_{k,4} x^k = \mathbb{O}(x)^4 - \sum_{k>0} \dim\ker{}^t\mathcal{C}_{k,4} x^k \le \mathbb{O}(x)^4 - 3\mathbb{O}(x)^2\mathbb{S}(x) + \mathbb{S}(x)^2$$

because of the identity (2.5) and the inequality (2.8). Theorem 1.2 follows from this and (2.18). We complete the proof of Theorem 1.2. $\square$

Remark. In general, we conjecture that the dimension of the kernel of the matrix $\mathcal{C}_{k,r}$ is given by

$$\dim\ker{}^t\mathcal{C}_{k,r} \overset{?}{=} \dim\ker{}^t\mathcal{E}_{k,r} + \sum_{1\le q\le r-2}\Big(\sum_{1<p<k}\operatorname{rank}\,\mathcal{C}_{p,q}\cdot\dim\ker{}^t\mathcal{E}_{k-p,r-q}\Big).$$

Then, by induction on r, the uneven part of motivic Broadhurst-Kreimer conjecture (2.17) follows from the (conjectural) equality $\sum_{k>0}\dim\ker\mathcal{E}_{k,r}x^k = \mathbb{O}(x)^{r-2}\mathbb{S}(x)$ (or equivalently, the surjectivity of the map $\mathcal{F}_{k,r}$ in Theorem 2.3).

4 Double Eisenstein series for $\Gamma_0(2)$ and modular forms

4.1 Double shuffle relation of double Eisenstein series for cusp ∞

We start with a brief introduction of the double shuffle relation of double Eisenstein series for $\Gamma_0(2)=\{(\begin{smallmatrix}a&b\\c&d\end{smallmatrix})\in\Gamma_1 \mid c\equiv 0 \pmod 2\}$. For integers $r\ge 3$ and $s\ge 2$ and $a,b\in\{0,1\}$ we define the double Eisenstein series $G^{(a,b)}_{r,s}(\tau)$ by

$$G^{(a,b)}_{r,s}(\tau) := \big(2\pi\sqrt{-1}\big)^{-r-s}\sum_{\substack{2m\tau+n>2m'\tau+n'>0\\ n\equiv a \mod 2\\ n'\equiv b \mod 2}}\frac{1}{(2m\tau+n)^r(2m'\tau+n')^s}. \tag{4.1}$$

For an integer $k\ge 3$ and $a\in\{0,1\}$, we define the function $G^{(a)}_k(\tau)$ by

$$G^{(a)}_k(\tau) = \big(2\pi\sqrt{-1}\big)^{-k}\sum_{\substack{2m\tau+n>0\\ n\equiv a \mod 2}}\frac{1}{(2m\tau+n)^k}. \tag{4.2}$$

Note that these give non-zero holomorphic functions on the upper half-plane even when k is odd. In particular, when $k\ge 4$ is even, the function $G^{(0)}_k(\tau)$ is the Eisenstein series for Γ_1 and the function $G^{(1)}_k(\tau)$ is the Eisenstein series for the congruence subgroup $\Gamma_0(2)$ associated to the cusp ∞. The product of these functions is expressible as a $\mathbb{Q}$-linear combination of double Eisenstein series. Indeed, for $r,s\ge 3$, we obtain

$$G_r^{(1)}(\tau)G_s^{(0)}(\tau) = G_{r,s}^{(1,0)}(\tau) + G_{s,r}^{(0,1)}(\tau),$$
$$G_r^{(1)}(\tau)G_s^{(1)}(\tau) = G_{r,s}^{(1,1)}(\tau) + G_{s,r}^{(1,1)}(\tau) + G_{r+s}^{(1)}(\tau).$$

This follows from the obvious decomposition of positive lattice points in $(\mathbb{Z}\tau+\mathbb{Z})\times(\mathbb{Z}\tau+\mathbb{Z})$ into three disjoint subsets $\{(m,n)\mid m>n\},\ \{(m,n)\mid m<n\}$ and $\{(m,n)\mid m=n\}$. On the other hand, the standard partial fraction decomposition

$$\frac{1}{x^r y^s} = \sum_{\substack{i+j=r+s\\ i,j\geq 1}} \left[\frac{\binom{i-1}{r-1}}{(x+y)^i x^j} + \frac{\binom{i-1}{s-1}}{(x+y)^i y^j}\right] \quad (r,s\in\mathbb{Z}_{>0})$$

deduces the different expressions

$$G_r^{(1)}(\tau)G_s^{(0)}(\tau) = \sum_{\substack{i+j=r+s\\ i,j\geq 1}} \left(\binom{i-1}{r-1}G_{i,j}^{(0,1)}(\tau) + \binom{i-1}{s-1}G_{i,j}^{(1,1)}(\tau)\right),$$
$$G_r^{(1)}(\tau)G_s^{(1)}(\tau) = \sum_{\substack{i+j=r+s\\ i,j\geq 1}} \left(\binom{i-1}{r-1} + \binom{i-1}{s-1}\right) G_{i,j}^{(0,1)}(\tau)$$

by letting $x = m\tau+n, y = m'\tau+n'$ and summing all positive lattice points on $\mathbb{Z}\tau+\mathbb{Z}$. These equalities give a collection of relations among double Eisenstein series, which we call the double shuffle relation. To complete these relations, we now give a regularization of the series $G_{r,s}^{(a,b)}(\tau)$ in (4.1) for any (non-converging) $r,s\geq 1$, by using q-series.

The constant term we use the double zeta values of level 2 defined by

$$\zeta^{(a,b)}(r,s) = \sum_{\substack{n_1>n_2>0\\ n_1\equiv a \mod 2\\ n_2\equiv b \mod 2}} \frac{1}{n_1^r n_2^s}.$$

We also need $\zeta^{(a)}(k) = \sum_{\substack{n>1\\ n\equiv a \mod 2}} n^{-k}$. By virtue of the regularization of the multiple L-values (see [1]), we put $\zeta^{(a)}(1) = \frac{1}{2}(T-(-1)^a\log 2)$, and for $s\geq 2$

$$\zeta^{(a,b)}(1,s) = \frac{1}{2}\zeta^{(b)}(s)T - \frac{(-1)^a}{2}(\log 2)\zeta^{(b)}(s) - \zeta^{(a,b)}(s,1) - \delta_{a,b}\zeta^{(a)}(s+1)$$

where T is a formal variable. We will write $\widetilde{\zeta}^{**}(r,s) = \zeta^{**}(r,s)/(2\pi\sqrt{-1})^{r+s}$. The following functions arise from the Fourier expansion of $G^{(a,b)}_{r,s}(\tau)$; for positive integers r,s and $a,b \in \{0,1\}$, set

$$g^{(a,b)}_{r,s}(q) = \frac{(-1)^{r+s}}{2^{r+s}(r-1)!(s-1)!} \sum_{\substack{m>m'>0\\ u,v>0}} (-1)^{au+bv} u^{r-1} v^{s-1} q^{um+vm'},$$

$$g^{(a)}_{r}(q) = \frac{(-1)^{r}}{2^{r}(r-1)!} \sum_{u,m>0} (-1)^{au} u^{r-1} q^{um},$$

and, for $k \geq 0$, let

$$\overline{g}^{(a)}_{k}(q) = \frac{(-1)^{k}}{2^{k+1}k!} \sum_{u,m>0} (-1)^{au} m u^{k} q^{um}.$$

For integers $r,s \geq 1$, we define

$$\varepsilon^{(a,b)}_{r,s}(q) = \delta_{r,2}\overline{g}^{(b)}_{s}(q) - \delta_{r,1}\overline{g}^{(b)}_{s-1}(q) + \delta_{s,1}(\overline{g}^{(a)}_{r-1}(q) + g^{(a)}_{r}(q)) + \delta_{r,1}\delta_{s,1}\alpha^{(a,b)}(q),$$

which is 0 when $r \geq 3$ and $s \geq 2$. Here we put

$$\alpha^{(0,1)}(q) = \overline{g}^{(1)}_{0}(q),\ \alpha^{(1,0)}(q) = -\alpha^{(0,1)},\ \alpha^{(1,1)}(q) = 2\overline{g}^{(1)}_{0}(q) + \overline{g}^{(0)}_{0}(q). \tag{4.3}$$

Remark. In the original paper [9], we took $\alpha^{(0,1)}(q) = \overline{g}^{(1)}_{0}(q) - \frac{1}{2}\overline{g}^{(0)}_{0}(q) = -\alpha^{(1,0)}(q)$ and $\alpha^{(1,1)}(q) = 4g^{(1)}_{2}(q) + \frac{1}{2}\overline{g}^{(0)}_{0}(q)$ instead of (4.3). This is incorrect, and was pointed out by Professor Jianqiang Zhao. The author would like to thank him.

Definition 4.1. *For integers $r,s \geq 1$ and $a,b \in \{0,1\}$ without $(r,s) = (1,1), (a,b) = (0,0)$, we define the regularized double Eisenstein series $G^{(a,b)}_{r,s}(q)$ by*

$$\begin{aligned} G^{(a,b)}_{r,s}(q) =& \widetilde{\zeta}^{(a,b)}(r,s) + g^{(a,b)}_{r,s}(q) + \frac{1}{4}\varepsilon^{(a,b)}_{r,s}(q) + g^{(a)}_{r}(q)\widetilde{\zeta}^{(b)}(s) \\ & + \sum_{\substack{p+h=k\\ p,h\geq 1}} \widetilde{\zeta}^{(a-b)}(p) \left((-1)^{s}\binom{p-1}{s-1} g^{(a)}_{h}(q) + (-1)^{p+r}\binom{p-1}{r-1} g^{(b)}_{h}(q) \right). \end{aligned}$$

(Note that when $r \geq 3$ and $s \geq 2$, each of regularized double Eisenstein series coincides with the defining series given in (4.1).) For $k \geq 1$, we also define the q-series $G^{(0)}_{k}(q)$

and $G_k^{(1)}(q)$ by

$$G_k^{(0)}(q) = \widetilde{\zeta}^{(0)}(k) + \frac{(-1)^k}{2^k(k-1)!}\sum_{n\geq 1}\sum_{d|n} d^{k-1}q^n,$$
$$G_k^{(1)}(q) = \widetilde{\zeta}^{(1)}(k) + \frac{(-1)^k}{2^k(k-1)!}\sum_{n\geq 1}\Big(\sum_{d|n}(-1)^d d^{k-1}\Big)q^n,$$

which coincide with the functions $G_k^{(0)}(\tau)$ and $G_k^{(1)}(\tau)$ when $k\geq 3$, respectively. Then the regularized double shuffle relation can be stated as follows:

Theorem 4.2. ([9]) *For any integers $r,s\geq 1$ and $a,b\in\{0,1\}$ with $(r,s)\neq(1,1)$ and $(a,b)\neq(0,0)$, we have*

$$\begin{aligned}
&G_r^{(a)}(q)G_s^{(b)}(q) + \frac{1}{4}(\delta_{r,2}\overline{g}_s^{(b)}(q) + \delta_{s,2}\overline{g}_r^{(a)}(q))\\
&= G_{r,s}^{(a,b)}(q) + G_{s,r}^{(b,a)}(q) + \delta_{a,b}G_{r+s}^{(a)}(q)\\
&= \sum_{\substack{i+j=r+s\\ i,j\geq 1}}\left(\binom{i-1}{r-1}G_{i,j}^{(a+b,b)}(q) + \binom{i-1}{s-1}G_{i,j}^{(a+b,a)}(q)\right).
\end{aligned}$$

Proof. As in [6], the proof of Theorem 4.2 is done by dividing into three parts: the constant term, the imaginary part, and the combinatorial part. We only prove the combinatorial part. Let $\beta_p^{(0)} = -\frac{B_p}{2^{p+1}p!}$ and $\beta_p^{(1)} = -\frac{(1-2^{-p})B_p}{2^{p+1}p!}$, and set

$$\beta_{r,s}^{(a,b)}(q) = g_r^{(a)}(q)\beta_s^{(b)} + \sum_{i+j=r+s}\beta_i^{(a-b)}\left((-1)^s\binom{i-1}{s-1}g_j^{(a)}(q) + (-1)^{i-r}\binom{i-1}{r-1}g_j^{(b)}(q)\right).$$

For integers $r,s\geq 1$, we define the combinatorial double Eisenstein series $\mathcal{G}_{r,s}^{(a,b)}(q)$ by

$$\mathcal{G}_{r,s}^{(a,b)}(q) = g_{r,s}^{(a,b)}(q) + \beta_{r,s}^{(a,b)}(q) + \frac{1}{4}\varepsilon_{r,s}^{(a,b)}(q).$$

Then, our task is to prove for all integers $r,s\geq 1$

$$\begin{aligned}
P_{r,s}^{(a,b)}(q) &= \mathcal{G}_{r,s}^{(a,b)}(q) + \mathcal{G}_{s,r}^{(b,a)}(q) + \delta_{a,b}\left(g_{r+s}^{(a)}(q) - \delta_{s,1}\delta_{r,1}\frac{\alpha^{(a,a)}}{2}\right)\\
&= \sum_{\substack{i+j=r+s\\ i,j\geq 1}}\left(\binom{i-1}{r-1}\mathcal{G}_{i,j}^{(a+b,b)}(q) + \binom{i-1}{s-1}\mathcal{G}_{i,j}^{(a+b,a)}(q)\right),
\end{aligned} \tag{4.4}$$

where $P^{(a,b)}_{r,s}(q) = g^{(a)}_r(q)g^{(b)}_s(q) + \beta^{(a)}_r g^{(b)}_s(q) + \beta^{(b)}_s g^{(a)}_r(q) + \frac{1}{4}\big(\delta_{r,2}\overline{g}^{(b)}_s(q) + \delta_{s,2}\overline{g}^{(a)}_r(q)\big)$. Consider their generating functions as follows:

$$\begin{aligned}
\mathcal{G}^{(1)}(X) &:= \sum_{k>0} g^{(1)}_k(q)X^{k-1} - \frac{\alpha^{(1,1)}(q)}{2}\cdot X,\\
\mathcal{G}^{(a,b)}(X,Y) &:= \sum_{r,s>0} \mathcal{G}^{(a,b)}_{r,s}(q)X^{r-1}Y^{s-1},\\
P^{(a,b)}(X,Y) &:= \sum_{r,s>0} P^{(a,b)}_{r,s}(q)X^{r-1}Y^{s-1}.
\end{aligned}$$

Then the relation (4.4) is equivalent to

$$\begin{aligned}
P^{(a,b)}(X,Y) &= \mathcal{G}^{(a,b)}(X,Y) + \mathcal{G}^{(b,a)}(Y,X) + \delta_{(a,b),(1,1)}\frac{\mathcal{G}^{(1)}(X) - \mathcal{G}^{(1)}(Y)}{X-Y} && (4.5)\\
&= \mathcal{G}^{(a+b,b)}(X+Y,Y) + \mathcal{G}^{(a+b,a)}(X+Y,X). && (4.6)
\end{aligned}$$

To prove this, we compute

$$\begin{aligned}
\beta^{(a)}(X) &:= \sum_{k>0}\beta^{(a)}_k X^{k-1} = -\frac{1}{4}\frac{1}{(-1)^a e^{X/2}-1} + \delta_{a,0}\frac{1}{2X},\\
g^{(a)}(X) &:= \sum_{k>0} g^{(a)}_k X^{k-1} = -\frac{1}{2}\sum_{u>0}(-1)^{au}e^{-\frac{uX}{2}}\cdot\frac{q^u}{1-q^u},\\
\overline{g}^{(a)}(X) &:= \sum_{k>0}\overline{g}^{(a)}_k X^{k-1} = \frac{1}{2X}\left(\sum_{u>0}(-1)^{au}e^{-\frac{uX}{2}}\cdot\frac{q^u}{(1-q^u)^2} - 2\overline{g}^{(a)}_0(q)\right),\\
g^{(a,b)}(X,Y) &:= \sum_{r,s>0} g^{(a,b)}_{r,s}X^{r-1}Y^{s-1}\\
&= \frac{1}{4}\sum_{u,b>0}(-1)^{au+bv}e^{-\frac{uX+vY}{2}}\cdot\frac{q^u}{1-q^u}\frac{q^{u+v}}{1-q^{u+v}},\\
\beta^{(a,b)}(X,Y) &:= \sum_{r,s>0}\beta^{(a,b)}_{r,s}(q)X^{r-1}Y^{s-1} = (g^{(b)}(Y)-g^{(a)}(X))\beta^{(a-b)}(X-Y) + g^{(a)}(X)\beta^{(b)}(Y),\\
\varepsilon^{(a,b)}(X,Y) &:= \sum_{r,s>0}\varepsilon^{(a,b)}_{r,s}(q)X^{r-1}Y^{s-1}\\
&= X\cdot\overline{g}^{(b)}(Y) - Y\cdot\overline{g}^{(b)}(X) + X\cdot\overline{g}^{(a)}(X) + g^{(a)}(X) - \overline{g}^{(b)}_0(q) + \overline{g}^{(a)}_0(q) + \alpha^{(a,b)}(q).
\end{aligned}$$

We note that the left-hand side of (4.5) can be written in the form

$$P^{(a,b)}(X,Y) = g^{(a)}(X)g^{(b)}(Y) + g^{(a)}(X)\beta^{(b)}(Y) + g^{(b)}(Y)\beta^{(a)}(X) + \frac{1}{4}\left(X\cdot\overline{g}^{(b)}(X) + Y\cdot\overline{g}^{(a)}(X)\right).$$

The right-hand side of (4.5) can be computed as follows:

$$\begin{aligned}
(\text{R.H.S. of (4.5)}) &= g^{(a,b)}(X,Y) + g^{(b,a)}(Y,X) + \beta^{(a,b)}(X,Y) + \beta^{(b,a)}(Y,X) \\
&+ \frac{1}{4}\varepsilon^{(a,b)}(X,Y) + \frac{1}{4}\varepsilon^{(b,a)}(Y,X) + \delta_{(a,b),(1,1)}\frac{\mathcal{G}^{(1)}(X) - \mathcal{G}^{(1)}(Y)}{X-Y} \\
&= g^{(a)}(X)g^{(b)}(Y) - \frac{1}{4}\big(g^{(a)}(X) + g^{(b)}(Y)\big) \\
&- \frac{1}{4}\big(g^{(a)}(X) - g^{(b)}(Y)\big)\cdot \coth\left(\frac{X - Y + 2\pi\sqrt{-1}(a-b)}{2}\right) \\
&+ g^{(a)}(X)\beta^{(b)}(Y) + g^{(b)}(Y)\beta^{(a)}(X) - \delta_{(a,b),(1,1)}\frac{g^{(1)}(X) - g^{(1)}(Y)}{X-Y} \\
&+ \frac{1}{4}\big(g^{(a)}(X) - g^{(b)}(Y)\big)\cdot \coth\left(\frac{X - Y + 2\pi\sqrt{-1}(a-b)}{2}\right) \\
&+ \frac{1}{4}\left(X\cdot \overline{g}^{(b)}(X) + Y\cdot \overline{g}^{(a)}(X) + g^{(a)}(X) + g^{(b)}(Y) + \alpha^{(a,b)}(q) + \alpha^{(b,a)}(q)\right) \\
&+ \delta_{(a,b),(1,1)}\left(\frac{g^{(1)}(X) - g^{(1)}(Y)}{X-Y} - \frac{\alpha^{(1,1)}}{2}\right) \\
&= P^{(a,b)}(X,Y).
\end{aligned}$$

For the right-hand side of (4.6), we can check

$$\begin{aligned}
&(\text{R.H.S. of (4.6)}) \\
&= g^{(a+b,b)}(X+Y,Y) + g^{(a+b,a)}(X+Y,X) + \beta^{(a+b,b)}(X+Y,Y) + \beta^{(a+b,a)}(X+Y,X) \\
&+ \frac{1}{4}\varepsilon^{(a+b,b)}(X+Y,Y) + \frac{1}{4}\varepsilon^{(a+b,a)}(X+Y,X) \\
&= g^{(a)}(X)g^{(b)}(Y) - \frac{X+Y}{2}\overline{g}^{(a+b)}(X+Y) - \frac{1}{2}\overline{g}_0^{(a+b)}(q) - \frac{1}{2}g^{(a+b)}(X+Y) \\
&+ g^{(a)}(Y)\beta^{(a)}(X) + g^{(a)}(X)\beta^{(b)}(Y) \\
&\frac{1}{4}\left(X\cdot \overline{g}^{(b)}(Y) + Y\cdot \overline{g}^{(a)}(X) + 2(X+Y)\overline{g}^{(a+b)}(X+Y) + 2g^{(a+b)}(X+Y)\right. \\
&\left. + 2\overline{g}_0^{(a+b)}(q) - \overline{g}_0^{(b)}(q) - \overline{g}_0^{(a)}(q) + \alpha^{(a+b,b)}(q) + \alpha^{(a+b,a)}(q)\right) \\
&= P^{(a,b)}(X,Y),
\end{aligned}$$

which complete the proof. $\square$

4.2 Formal double shuffle space for level 2

In [9], we proved that the space spanned by double Eisenstein series $G^{(1,1)}_{2i,k-2i}(q)$ $(2 \le i \le k/2-1)$ contains the space of cusp forms on $\Gamma_0(2)$. We now give a proof of this result. The proof it is important to study the formal double shuffle space, which was first considered by Gangl, Kaneko and Zagier [6] in the case of Γ_1.

Let $k > 2$ and $\mathcal{DZ}_k$ be the $\mathbb{Q}$-vector space spanned by formal symbols $Z^{\mathbf{eo}}_{r,s}, Z^{\mathbf{oe}}_{r,s}$, $Z^{\mathbf{oo}}_{r,s}$, $P^{\mathbf{oe}}_{r,s}$, $P^{\mathbf{oo}}_{r,s}$ $(r, s \ge 1,\ r+s=k)$, and $Z^{\mathbf{o}}_k$ with the set of relations

$$P^{\mathbf{oe}}_{r,s} = Z^{\mathbf{oe}}_{r,s} + Z^{\mathbf{eo}}_{s,r} = \sum_{\substack{i+j=k\\ i,j\ge 1}} \left(\binom{i-1}{r-1} Z^{\mathbf{oe}}_{i,j} + \binom{i-1}{s-1} Z^{\mathbf{oo}}_{i,j} \right), \tag{4.7}$$

$$P^{\mathbf{oo}}_{r,s} = Z^{\mathbf{oo}}_{r,s} + Z^{\mathbf{oo}}_{s,r} + Z^{\mathbf{o}}_k = \sum_{\substack{i+j=k\\ i,j\ge 1}} \left(\binom{i-1}{r-1} + \binom{i-1}{s-1} \right) Z^{\mathbf{eo}}_{i,j} \tag{4.8}$$

for $r, s \ge 1$, $r+s=k$, so that

$$\mathcal{DZ}_k = \frac{\{\mathbb{Q}\text{-linear combinations of } Z^{\mathbf{eo}}_{r,s}, Z^{\mathbf{oe}}_{r,s}, Z^{\mathbf{oo}}_{r,s}, P^{\mathbf{oe}}_{r,s}, P^{\mathbf{oo}}_{r,s}, Z^{\mathbf{o}}_k\}}{\langle \mathbb{Q}\text{-linear span of relations } (4.7), (4.8)\rangle}.$$

Since the elements $P^{\mathbf{oe}}_{r,s}$ and $P^{\mathbf{oo}}_{r,s}$ are written in Z's, we can also regard the space as given by

$$\mathcal{DZ}_k = \frac{\{\mathbb{Q}\text{-linear combinations of } Z^{\mathbf{eo}}_{r,s}, Z^{\mathbf{oe}}_{r,s}, Z^{\mathbf{oo}}_{r,s}, Z^{\mathbf{o}}_k\}}{\langle \mathbb{Q}\text{-linear span of relations } (4.9), (4.10)\rangle}$$

where the defining relations (4.9) and (4.10) are

$$Z^{\mathbf{oe}}_{r,s} + Z^{\mathbf{eo}}_{s,r} = \sum_{\substack{i+j=k\\ i,j\ge 1}} \left(\binom{i-1}{r-1} Z^{\mathbf{oe}}_{i,j} + \binom{i-1}{s-1} Z^{\mathbf{oo}}_{i,j} \right), \tag{4.9}$$

$$Z^{\mathbf{oo}}_{r,s} + Z^{\mathbf{oo}}_{s,r} + Z^{\mathbf{o}}_k = \sum_{\substack{i+j=k\\ i,j\ge 1}} \left(\binom{i-1}{r-1} + \binom{i-1}{s-1} \right) Z^{\mathbf{eo}}_{i,j}. \tag{4.10}$$

Note that the relations (4.7) and (4.8) (as well as (4.9) and (4.10)) correspond to those in Theorem 4.2, under the correspondences

$$
\begin{aligned}
Z^{\mathbf{eo}}_{r,s} \longleftrightarrow G^{(0,1)}_{r,s}(q), \quad Z^{\mathbf{oe}}_{r,s} \longleftrightarrow G^{(1,0)}_{r,s}(q), \quad Z^{\mathbf{oo}}_{r,s} \longleftrightarrow G^{(1,1)}_{r,s}(q), \quad Z^{\mathbf{o}}_{k} \longleftrightarrow G^{(1)}_{k}(q),\\
P^{\mathbf{oe}}_{r,s} \longleftrightarrow G^{(1)}_{r}(q)G^{(0)}_{s}(q) + \frac{1}{4}(\delta_{r,2}\overline{g}^{(0)}_{s}(q) + \delta_{s,2}\overline{g}^{(1)}_{r}(q)) \qquad (4.11)\\
P^{\mathbf{oo}}_{r,s} \longleftrightarrow G^{(1)}_{r}(q)G^{(1)}_{s}(q) + \frac{1}{4}(\delta_{r,2}\overline{g}^{(1)}_{s}(q) + \delta_{s,2}\overline{g}^{(1)}_{r}(q)).
\end{aligned}
$$

Theorem 4.3. ([9, Theorem 1]) *Suppose k is even and $k \geq 4$. In $\mathcal{DZ}_k$, we have*
(i)

$$\sum_{\substack{r=2\\ r:\text{even}}}^{k-2} Z^{\mathbf{oo}}_{r,k-r} = \frac{1}{4} Z^{\mathbf{o}}_{k}. \tag{4.12}$$

(ii) Each $P^{\mathbf{oe}}_{r,k-r}$ with r even can be written as a $\mathbb{Q}$-linear combination of $P^{\mathbf{oo}}_{i,j}$ $(i,j:\text{even}, i+j=k)$ and $Z^{\mathbf{o}}_{k}$

Proof. Consider the generating functions

$$
\begin{aligned}
\mathfrak{Z}^{\mathbf{eo}}_{k}(X,Y) &= \sum_{r+s=k} Z^{\mathbf{eo}}_{r,s} X^{r-1}Y^{s-1},\ \mathfrak{Z}^{\mathbf{oe}}_{k}(X,Y) = \sum_{r+s=k} Z^{\mathbf{oe}}_{r,s} X^{r-1}Y^{s-1},\\
\mathfrak{Z}^{\mathbf{oo}}_{k}(X,Y) &= \sum_{r+s=k} Z^{\mathbf{oo}}_{r,s} X^{r-1}Y^{s-1}.
\end{aligned}
$$

Here and in the following, the sum $\sum_{r+s=k}$ always means $\sum_{r+s=k,\, r,s\geq 1}$. The double shuffle relations (4.9) and (4.10) are equivalent to the relations

$$\mathfrak{Z}^{\mathbf{oe}}_{k}(X,Y) + \mathfrak{Z}^{\mathbf{eo}}_{k}(Y,X) = \mathfrak{Z}^{\mathbf{oe}}_{k}(X+Y,Y) + \mathfrak{Z}^{\mathbf{oo}}_{k}(X+Y,X), \tag{4.13}$$

$$\mathfrak{Z}^{\mathbf{oo}}_{k}(X,Y) + \mathfrak{Z}^{\mathbf{oo}}_{k}(Y,X) + Z^{\mathbf{o}}_{k} \cdot \frac{X^{k-1}-Y^{k-1}}{X-Y} = \mathfrak{Z}^{\mathbf{eo}}_{k}(X+Y,Y) + \mathfrak{Z}^{\mathbf{eo}}_{k}(X+Y,X). \tag{4.14}$$

Substituting $X=1, Y=0$ in (4.13) and $X=1, Y=-1$ in (4.14), we respectively obtain

$$Z^{\mathbf{oe}}_{k-1,1} + Z^{\mathbf{eo}}_{1,k-1} = Z^{\mathbf{oe}}_{k-1,1} + \sum_{r=1}^{k-1} Z^{\mathbf{oo}}_{r,k-r}, \tag{4.15}$$

$$2\sum_{r=1}^{k-1}(-1)^{r-1} Z^{\mathbf{oo}}_{r,k-r} + Z^{\mathbf{o}}_{k} = 2Z^{\mathbf{eo}}_{1,k-1}. \tag{4.16}$$

We divide (4.16) by 2 and add (4.15) to obtain

$$\frac{1}{2}Z_k^{\mathbf{o}} = 2\sum_{\substack{r=2\\ r:\,even}}^{k-2} Z_{r,k-r}^{\mathbf{oo}}$$

and hence (i) of Theorem.

To prove (ii), we need the following lemma.

Lemma 4.4. *Let $k \geq 4$ be an even integer and $a_{i,j}, b_{i,j}, c_{i,j}$ be rational numbers. Then the following two statements are equivalent.*

1) The relation

$$\sum_{i+j=k} a_{i,j} Z_{i,j}^{\mathbf{eo}} + \sum_{i+j=k} b_{i,j} Z_{i,j}^{\mathbf{oe}} + \sum_{i+j=k} c_{i,j} Z_{i,j}^{\mathbf{oo}} \equiv 0 \pmod{\mathbb{Q}Z_k^{\mathbf{o}}}$$

holds in $\mathcal{DZ}_k$ (as before $\sum_{i+j=k}$ means $\sum_{i+j=k,\, i,j\geq 1}$).

2) There exist some homogeneous polynomials $F, G \in \mathbb{Q}[X,Y]$ of degree $k-2$ such that

$$\begin{aligned} &F(Y_1,X_1)+F(X_2,Y_2)-F(X_2,X_2+Y_2)-F(X_3+Y_3,X_3)\\ &+G(X_3,Y_3)+G(Y_3,X_3)-G(X_1,X_1+Y_1)-G(X_1+Y_1,X_1)\\ &=\sum_{i+j=k}\binom{k-2}{i-1}a_{i,j}X_1^{i-1}Y_1^{j-1}+\sum_{i+j=k}\binom{k-2}{i-1}b_{i,j}X_2^{i-1}Y_2^{j-1}+\sum_{i+j=k}\binom{k-2}{i-1}c_{i,j}X_3^{i-1}Y_3^{j-1}. \end{aligned}$$

Proof. This is an analogue of Proposition 5.1 in [6]. Take $F(X,Y) = \binom{k-2}{r-1}X^{r-1}Y^{s-1}$ (and $G=0$) and compute the coefficients of $F(Y_1,X_1)+F(X_2,Y_2)-F(X_2,X_2+Y_2)-F(X_3+Y_3,X_3)$ using binomial theorem. Then the relation in 1) is exactly (not only mod $\mathbb{Q}Z_k^{\mathbf{o}}$ but as an exact equality) the relation (4.9). Similarly, by taking $G(X,Y) = \binom{k-2}{r-1}X^{r-1}Y^{s-1}$ (and $F=0$) and computing the coefficients of $G(X_3,Y_3)+G(Y_3,X_3)-G(X_1,X_1+Y_1)-G(X_1+Y_1,X_1)$, we see that the relation in 1) is the relation (4.10) modulo $\mathbb{Q}Z_k^{\mathbf{o}}$. Since any relation of the form in 1) in $\mathcal{DZ}_k$ should come from a linear combination of (4.9) and (4.10) modulo $\mathbb{Q}Z_k^{\mathbf{o}}$, and any homogeneous polynomial is a linear combination of monomials, we obtain the lemma. □

Using the lemma, we are going to produce enough relations of the form

$$\sum_{\substack{r+s=k\\ r,s:\,\text{even}}} \alpha_{r,s} P_{r,s}^{\mathbf{oe}} \equiv \sum_{\substack{r+s=k\\ r,s:\,\text{even}}} \beta_{r,s} P_{r,s}^{\mathbf{oo}} \pmod{\mathbb{Q}Z_k^{\mathbf{o}}} \tag{4.17}$$

such that we can solve these in $P^{\mathbf{oe}}_{r,s}$. In view of the relations

$$P^{\mathbf{oe}}_{r,s} = Z^{\mathbf{oe}}_{r,s} + Z^{\mathbf{eo}}_{s,r},\ P^{\mathbf{oo}}_{r,s} \equiv Z^{\mathbf{oo}}_{r,s} + Z^{\mathbf{oo}}_{s,r} \pmod{\mathbb{Q}Z^{\mathbf{o}}_k} \tag{4.18}$$

and the lemma, we obtain the relation of the form (4.17) if we can take F and G in 2) of Lemma 4.4 so that the coefficients satisfy

(i) $a_{i,j} = b_{j,i}$,

(ii) $c_{i,j} = c_{j,i}$,

(iii) $a_{i,j} = b_{i,j} = c_{i,j} = 0$ for all odd i, j.

We now work for convenience with inhomogeneous polynomials. Recall the usual correspondences $f(x) = F(x,1)$ and $F(X,Y) = Y^{k-2}f(X/Y)$, and the action of the group $\Gamma = \mathrm{PGL}_2(\mathbb{Z})$ on the space of polynomials of degree at most $k-2$ by (we are assuming k is even)

$$f(x)\Big|_{k-2}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = (cx+d)^{k-2} f\left(\frac{ax+b}{cx+d}\right). \tag{4.19}$$

We extend this action to the group ring $\mathbb{Z}[\Gamma]$ by linearity. Set

$$T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix},\ S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ \delta = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},\ \varepsilon = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then the left-hand side of the equation in 2) of Lemma 4.4 can be written in inhomogeneous form as

$$\big(f\big|\varepsilon - g\big|(TST + TS\delta)\big)(x_1) + \big(f\big|(1-TST)\big)(x_2) - \big(f\big|TS\delta - g\big|(1+\varepsilon)\big)(x_3). \tag{4.20}$$

(We write $\big|$ instead of $\big|_{k-2}$.)

Lemma 4.5. *Suppose the polynomial $f(x)$ (of degree at most $k-2$) satisfies $f\big|TST\delta = f$ and put $g = \frac{1}{2}f\big|T\delta$. Then the expression* (4.20) *gives the coefficients satisfying the above three conditions (i), (ii), (iii).*

Proof. Inserting $g = \frac{1}{2}f\big|T\delta$ into (4.20) and using the assumption $f\big|TST\delta = f$, which is equivalent to $f\big|TS = f\big|T\delta$ since $(T\delta)^2 = 1$, and also using the identities $TSTST =$

$S, T\delta T = \delta, \delta S = \varepsilon, \varepsilon\delta = \delta\varepsilon = S$ in Γ, we can write (4.20) as

$$\left(f\big|\varepsilon(1-\delta)\right)(x_1) + \left(f\big|(1-\delta)\right)(x_2) - \left(f\big|T(1-\delta)\right)(x_3). \tag{4.21}$$

Now the condition (iii) (the polynomial is even) is clear from this (being killed by $1+\delta$), and the conditions (i) and (ii) are respectively the consequences of the equations

$$\begin{aligned}
&f\big|\varepsilon(1-\delta)\varepsilon = f\big|(1-\delta),\\
&f\big|T(1-\delta)\varepsilon = f\big|T\varepsilon - f\big|TS = f\big|T\delta S - f\big|T\delta = f\big|T(1-\delta).
\end{aligned}$$

$\square$

Noting $TST\delta = \left(\begin{smallmatrix}-1 & 0\\ -1 & 1\end{smallmatrix}\right)$ and hence

$$(-x+1)\left(\frac{-x}{-x+1}\right) = -x, \quad \text{and} \quad (-x+1)\left(\frac{-x}{-x+1} - 2\right) = x-2,$$

we see that the polynomials $x^r(x-2)^{k-2-r}$ for $r = 0, 2, \ldots, k-2$ (even) satisfy the condition $f\big|TST\delta = f$ in Lemma 4.5. With this choice of f (for $r = 0, 2, \ldots, k-4$) and g in Lemma 4.5, we compute the coefficients in Lemma 4.4 by noting (4.18), (4.21) and by using

$$\begin{aligned}
&x^r(x-2)^{k-2-r}|(1-\delta) = x^r(x-2)^{k-2-r} - x^r(x+2)^{k-2-r}\\
&= -\sum_{\substack{i=1\\ i:odd}}^{k-2-r-1} \binom{k-2-r}{i} 2^{k-1-r-i} x^{r+i}\\
&= -\sum_{\substack{i=r+2\\ i:even}}^{k-2} \binom{k-2-r}{i-1-r} 2^{k-i} x^{i-1} \qquad (r+i \to i-1)\\
&= -\binom{k-2}{r}^{-1} \sum_{\substack{i=r+2\\ i:even}}^{k-2} \binom{k-2}{i-1}\binom{i-1}{r} 2^{k-i} x^{i-1},
\end{aligned}$$

to obtain a relation of the form

$$\sum_{\substack{i=r+2\\ i:even}}^{k-2} \binom{i-1}{r} 2^{k-i} P^{\mathbf{oe}}_{i,k-i} \equiv \text{linear combination of } P^{\mathbf{oo}}_{\text{even,even}} \pmod{\mathbb{Q}Z^{\mathbf{o}}_k}.$$

When we put $r = k-4, \ldots, 2, 0$, we can solve these congruences successively in each

$P^{\mathbf{oe}}_{i,k-i}$ for $i = k-2, k-4, \dots, 2$ (because the system is triangular). This completes the proof of Theorem 4.3.

□

Combining the first equality of (4.8) with (4.12), we have

$$(1 + 4 \cdot [k/4]) Z^{\mathbf{o}}_k = 2 \sum_{r=1}^{[k/4]} (2 - \delta_{r,k/4}) P^{\mathbf{oo}}_{2r,k-2r}.$$

Then, for even $k \geq 4$, as a consequence of Theorem 4.3, we find

$$\langle P^{\mathbf{oe}}_{2r,k-2r}, P^{\mathbf{oo}}_{2r,k-2r}, Z^{\mathbf{o}}_k \mid 1 \leq r \leq k/2 - 1 \rangle_{\mathbb{Q}} = \langle P^{\mathbf{oo}}_{2r,k-2r}, Z^{\mathbf{o}}_k \mid 2 \leq r \leq [k/4] \rangle_{\mathbb{Q}}. \quad (4.22)$$

Theorem 4.6. [9, Theorem 5] *Let $k \geq 4$ be a positive even integer and set $\mathcal{DE}^{(\infty)}_k = \big\langle G^{(1,1)}_{2i,k-2i}(q) \mid 1 \leq i \leq k/2 - 1 \big\rangle_{\mathbb{Q}}$.*
(i) Then the space $\mathcal{DE}^{(\infty)}_k$ contains $\mathbb{Q} \cdot G^{(1)}_k(q) \oplus S^{\mathbb{Q}}_k(2)$, where $S^{\mathbb{Q}}_k(2)$ is the $\mathbb{Q}$-vector space of cusp forms having rational Fourier coefficients.
(ii)

$$\dim \mathcal{DE}^{(\infty)}_k = \frac{k}{2} - 1,$$

so that the series $G^{(1,1)}_{r,k-r}(q)$ (r even) are linearly independent over $\mathbb{Q}$.

Proof. We first prove (i). For $k \geq 1$, define

$$E^{(1)}_k(q) = 2^k \big(G^{(0)}_k(q) - G^{(0)}_k(q^2) \big) = \frac{(-1)^k}{(k-1)!} \sum_{n \geq 1} \Big(\sum_{\substack{d \mid n \\ n/d:odd}} d^{k-1} \Big) q^n.$$

Note that when $k \geq 4$ is even, the q-series $E^{(1)}_k(q)$ is the Eisenstein series on $\Gamma_0(2)$ associated to the cusp 0 (this notation might cause confusion, but it works for the double Eisenstein series for the cusp 0). By the theorem of Imamoḡlu and Kohnen [8], it is known that the products $E^{(1)}_{2l}(q) G^{(1)}_{k-2l}(q)$ ($l = 2, 3, \dots, k/2 - 2$) generate $S^{\mathbb{Q}}_k(2)$. Note that each generators $E^{(1)}_{2l}(q) G^{(1)}_{k-2l}(q)$ ($l = 2, 3, \dots, k/2-2$) can be written in the form

$$E^{(1)}_{2l}(q) G^{(1)}_{k-2l}(q) = (2^{2l} - 1) G^{(0)}_{2l}(q) G^{(1)}_{k-2l}(q) - G^{(1)}_{2l}(q) G^{(1)}_{k-2l}(q).$$

With (4.22) and (4.11), we have

$$E^{(1)}_{2l}(q) G^{(1)}_{k-2l}(q) \in \langle G^{(1)}_k(q), G^{(1)}_{2l}(q) G^{(1)}_{k-2l} \mid 2 \leq l \leq [k/4] \rangle_{\mathbb{Q}},$$

and from (4.12) we find

$$G_k^{(1)}(q) \in \mathcal{DE}_k^{(\infty)}.$$

This implies that the space $\mathcal{DE}_k^{(\infty)}$ contains the space $\mathbb{Q} \cdot G_k^{(1)}(q) \oplus S_k^{\mathbb{Q}}(2)$.

For (ii), first we note by definition the inequality

$$\dim \mathcal{DE}_k^{(\infty)} \leq \frac{k}{2} - 1.$$

Since elements in $\mathbb{Q} \cdot G_k^{(1)}(q) \oplus S_k^{\mathbb{Q}}(2)$ have no imaginary parts, they sit in the kernel of the projection π from $\mathcal{DE}_k^{(\infty)}$ to $\sqrt{-1}\mathbb{R}[[q]]$, thus

$$\dim \ker \pi \geq 1 + \dim S_k(2) = \left[\frac{k}{4}\right].$$

Recalling (2.1), we have

$$\pi\big(G_{k_1,k_2}^{(1,1)}(q)\big) = \sum_{\substack{s_1+s_2=k_1+k_2 \\ s_1 \geq 3:\text{odd}}} \varepsilon_{\binom{s_1,s_2}{k_1,k_2}} \widetilde{\zeta}^{(0)}(s_1) g_{s_2}^{(1)}(q).$$

Then, as for the dimension of the image of π, we see that it is equal to the rank of the matrix

$$\mathcal{A}_{k,2} = \Big(\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}\Big)_{\substack{(s_1,s_2) \in S_{k,2} \\ k_1+k_2=k,\, k_1,k_2 \geq 2:\text{even}}}$$

because the series $g_3^{(1)}(q), g_5^{(1)}(q), \ldots, g_{k-3}^{(1)}(q)$ are linearly independent over $\mathbb{C}$. This can be seen as follows. For an odd prime p, the coefficient of q^p in $g_r^{(1)}(q)$ is $1 + p^{r-1}$ times a constant independent of p. Hence by picking distinct odd prime numbers $p_3, p_5, \ldots, p_{k-5}$ and looking at the coefficients of $q, q^{p_3}, q^{p_5}, \ldots, q^{p_{k-5}}$ in $g_3^{(1)}(q), g_5^{(1)}(q), \ldots, g_{k-3}^{(1)}(q)$, we see the desired linear independence because the coefficient matrix is essentially the (non-vanishing) Vandermonde determinant. We thus have

$$\dim \operatorname{im} \pi = \operatorname{rank} \mathcal{A}_{k,2} = \left[\frac{k+2}{4}\right] - 1,$$

where we postpone a computation of rank $\mathcal{A}_{k,2}$ to Section 5.1 (see (5.1)). This shows

$$\dim \mathcal{DE}_k^{(\infty)} \geq \left[\frac{k}{4}\right] + \left[\frac{k+2}{4}\right] - 1 = \frac{k}{2} - 1.$$

Therefore we conclude

$$\dim \mathcal{DE}_k^{(\infty)} = \frac{k}{2} - 1$$

and also

$$\ker \pi = \mathbb{Q} \cdot G_k^{(1)}(q) \oplus S_k^{\mathbb{Q}}(2).$$

□

Corollary 4.7. *For an even integer $k > 2$, we have*

$$\dim\langle \zeta^{\mathbf{oo}}(2r, k-2r) \mid 1 \leq r \leq k/2 - 1\rangle_{\mathbb{Q}} \leq \frac{k}{2} - 1 - \dim S_k(2).$$

Proof. By taking the constant term of the q-series, we obtain the surjective map

$$\mu : \mathcal{DE}_k^{(\infty)} \longrightarrow \langle \zeta^{\mathbf{oo}}(2r, k-2r) \mid 1 \leq r \leq k/2 - 1\rangle_{\mathbb{Q}}.$$

By the theorem, the kernel of μ contains the space $S_k^{\mathbb{Q}}(2)$ and hence we obtain the corollary. □

We end this subsection with the following theorem. Let $M_k^{\mathbb{Q}}(2)$ be the $\mathbb{Q}$-vector space spanned by modular forms whose Fourier coefficients are rational number of weight k on $\Gamma_0(2)$. We obtain bases of the space $M_k^{\mathbb{Q}}(2)$.

Theorem 4.8. *Recall that when $k > 3$ is even, the q-series $G_k^{(1)}(q)$ and $E_k^{(1)}(q)$ are the Eisenstein series of weight k on $\Gamma_0(2)$ associated to the cusps ∞ and 0 respectively.*
(i) For each positive even integer $k \geq 4$, the set

$$\{G_k^{(1)}(q), E_k^{(1)}(q), G_{2l}^{(1)}(q)G_{k-2l}^{(1)}(q) \mid 2 \leq l \leq [k/4]\}$$

forms a basis of the space $M_k^{\mathbb{Q}}(2)$.
(ii) For each positive even integer $k \geq 4$, the set

$$\{G_k^{(1)}(q), E_k^{(1)}(q), E_{2l}^{(1)}(q)E_{k-2l}^{(1)}(q) \mid 2 \leq l \leq [k/4]\}$$

forms a basis of the space $M_k^{\mathbb{Q}}(2)$.

Proof. We first prove (i). In the proof of Theorem 4.6, we showed that the space $S_k^{\mathbb{Q}}(2)$ is contained in the space spanned by the set $\{G_k^{(1)}(q), E_k^{(1)}(q), G_{2l}^{(1)}(q)G_{k-2l}^{(1)}(q) \mid 2 \leq l \leq [k/4]\}$. Then the assertion follows immediately from $\dim M_k^{\mathbb{Q}}(2) = [k/4] + 1$ and $M_k^{\mathbb{Q}}(2) = \mathbb{Q}\cdot G_k^{(1)}(q) \oplus \mathbb{Q}\cdot E_k^{(1)}(q) \oplus S_k^{\mathbb{Q}}(2)$. We note that the Fricke involution W_2 induces an endomorphism of $M_k^{\mathbb{Q}}(2)$. Then the basis (ii) follows from the transformation formula

$$E_k^{(1)}(q)\big|W_2\big(:= (2\tau)^{-k}E_k^{(1)}(\frac{-1}{2\tau})\big) = G_k^{(1)}(q) \quad (k \geq 4 : \text{even}). \tag{4.23}$$

$\square$

4.3 Application to Chan and Chua Conjecture

Theorem 4.8 has an application to solving one of the conjectures proposed by Chan and Chua [5]. We begin with stating this conjecture. Let

$$\theta(q) = \sum_{n\in\mathbb{Z}} q^{n^2}$$

be the standard theta function. We define three modular forms $G_{2k,4}(q)$, $F_{2k}(q)$ and $H_{2k+1}(q)$ by

$$\begin{aligned}
&G_{2k,4}(q) = G_{2k}^{(1)}(-q),\ F_{2k}(\tau) = G_{2k,4}(q) - 2G_{2k,4}(q^2),\\
&H_{2k+1}(q) = c_k - 4(-1)^k\sum_{n>0}\left(\frac{(2n)^{2k}q^n}{1+q^{2n}} + \frac{(-1)^n(2n-1)^{2k}q^{2n-1}}{1-q^{2n-1}}\right),
\end{aligned}$$

where the rational number c_k is defined as $\sec x = \sum_{k\geq 0} c_k\frac{x^{2k}}{(2k)!}$. These satisfy

$$G_{2k,4}(q) \in M_{2k}(4)\ (k \geq 2),\ F_{2k}(q) \in M_{2k}(4)\ (k \geq 1),\ H_{2k+1}(q) \in M_{2k+1}(4,\chi_4)\ (k \geq 1),$$

where χ_4 is the non-trivial character of conductor 4.

Conjecture 4.9. (Chan-Chua [5]) *For each positive integer $s \geq 2$, we have*

$$\begin{aligned}
&\theta(q)^{8s} \overset{?}{=} \sum_{l=2}^{s}\alpha_l G_{2l,4}(q)G_{4s-2l,4}(q),\ \theta(q)^{8s+4} \overset{?}{=} \sum_{l=1}^{s}\beta_l F_{2l}(q)G_{4s-2l,4}(q),\\
&\theta(q)^{8s+2} \overset{?}{=} \sum_{l=1}^{s}\gamma_l H_{2l+1}(q)F_{4s-2l}(q),\ \theta(q)^{8s+6} \overset{?}{=} \sum_{l=1}^{s}\delta_l H_{2l+1}(q)G_{4s-2l+2,4}(q),
\end{aligned}$$

for some $\alpha_l, \beta_l, \gamma_l, \delta_l \in \mathbb{Q}$.

In [14], the author has succeeded in proving the formulas on $\theta(q)^{8s}$ in Conjecture 4.9.

Theorem 4.10. *For any positive integer $s \geq 2$, there exist unique rational numbers $\mu_s(l)$ $(l = 2, 3, \ldots, s)$ such that*

$$\theta(q)^{8s} = 2^{8s} \sum_{l=2}^{s} \mu_s(l) G_{2l}^{(1)}(-q) G_{4s-2l}^{(1)}(-q). \tag{4.24}$$

Proof. Let

$$T(q) = q^{1/8} \sum_{n \geq 0} q^{n(n+1)/2}.$$

We note that for each positive integer s, the q-series $T(q)^{8s}$ is a modular form of weight k on $\Gamma_0(2)$, and hence is an element of the space $\mathbb{Q} \cdot E_{4s}^{(1)}(q) \oplus S_{4s}^{\mathbb{Q}}(2)$ because $\mathrm{ord}_{q=0} T(q)^{8s} > 0$, where $\mathrm{ord}_{q=0} f(q)$ is the vanishing order of $f(q)$ at $q = 0$. Then, from Theorem 4.8 (ii), there exist unique rational numbers $\alpha, \mu_s(l)$ $(l = 2, 3, \ldots, s)$ such that

$$T(q)^{8s} = \alpha E_{4s}^{(1)}(q) + \sum_{l=2}^{s} \mu_s(l) E_{2l}^{(1)}(q) E_{4s-2l}^{(1)}(q).$$

Since $\mathrm{ord}_\infty T(q)^{8s} = s \geq 2, \mathrm{ord}_\infty E_{4s}^{(1)}(q) = 1$ and $\mathrm{ord}_\infty E_{2l}^{(1)}(q) E_{4s-2l}^{(1)}(q) = 2$ $(2 \leq l \leq s)$, we find that $\alpha = 0$. Thus, we have unique expression of $T(q)^{8s}$ as follows.

$$T(q)^{8s} = \sum_{l=2}^{s} \mu_s(l) E_{2l}^{(1)}(q) E_{4s-2l}^{(1)}(q). \tag{4.25}$$

Thereby, using the transformation formulas

$$T(q)^{8s} \big| W_2 = \theta(-q)^{8s} \quad (s \geq 1)$$

and (4.23), the formulas (4.24) is easily deduced from (4.25). We indeed have

$$\begin{aligned}
\theta(-q)^{8s} \big(= 2^{8s}(2\tau)^{-4s} T(-\frac{1}{2\tau})^{8s}\big) &= 2^{8s}(2\tau)^{-4s} \sum_{l=2}^{s} \mu_s(l) E_{2l}^{(1)}(-\frac{1}{2\tau}) E_{4s-2l}^{(1)}(-\frac{1}{2\tau}) \\
&= 2^{8s} \sum_{l=2}^{s} \mu_s(l) G_{2l}^{(1)}(q) G_{4s-2l}^{(1)}(q),
\end{aligned}$$

and, hence, we obtain (4.24) by letting $q \to -q$. $\square$

4.4 Double shuffle relation of double Eisenstein series for cusp 0

In this section, we construct the double Eisenstein series for $\Gamma_0(2)$ associated to the cusp 0: its series expression is given by

$$E_{r,s}^{(a,b)}(\tau) = \left(2\pi\sqrt{-1}\right)^{-r-s} \sum_{\substack{m\tau+n > m'\tau+n' > 0 \\ m \equiv a \mod 2 \\ m' \equiv b \mod 2}} \frac{1}{(m\tau+n)^r (m'\tau+n')^s}. \tag{4.26}$$

We now describe a regularization of the double Eisenstein series $E_{r,s}^{(a,b)}(\tau)$ by using q-series. We begin with computing its Fourier expansion. For $k \geq 1$, we set

$$\varphi_k(q) = \frac{(-1)^k}{(k-1)!} \sum_{u>0} u^{k-1} q^u.$$

Proposition 4.11. *For any integers $r \geq 3$ and $s \geq 2$, we have*

$$\begin{aligned}
E_{r,s}^{(0,1)}(\tau) &= \sum_{\substack{m>m'>0 \\ m\equiv 0, m'\equiv 1}} \varphi_r(q^m)\varphi_s(q^{m'}), \\
E_{r,s}^{(1,0)}(\tau) &= \sum_{\substack{m>m'>0 \\ m\equiv 1, m'\equiv 0}} \varphi_r(q^m)\varphi_s(q^{m'}) + \widetilde{\zeta}(s) \sum_{m>0:\mathrm{odd}} \varphi_r(q^m), \\
E_{r,s}^{(0,0)}(\tau) &= \sum_{\substack{m>m'>0 \\ m\equiv 1, m'\equiv 1}} \varphi_r(q^m)\varphi_s(q^{m'}) \\
&\quad + \sum_{\substack{p+h=r+s \\ p,h\geq 1}} \left((-1)^s \binom{p-1}{s-1} + (-1)^{p+r}\binom{p-1}{r-1}\right) \widetilde{\zeta}(p) \sum_{m>0:\mathrm{odd}} \varphi_h(q^m).
\end{aligned}$$

Proof. We first recall the Lipschitz formula

$$\begin{aligned}
\lim_{N\to\infty} \sum_{n=-N}^{N} \frac{1}{\tau+n} &= -\pi\sqrt{-1} + (-2\pi\sqrt{-1}) \sum_{u>0} q^u = -\pi i + 2\pi\sqrt{-1}\varphi_1(q), \\
\sum_{n\in\mathbb{Z}} \frac{1}{(\tau+n)^r} &= \frac{(-2\pi\sqrt{-1})^r}{(r-1)!} \sum_{u>0} u^{r-1} q^u = (2\pi\sqrt{-1})^r \varphi_r(q) \quad (r \geq 2).
\end{aligned}$$

We can divide the summation in the defining series (4.26) into four terms, corresponding to $m = m' = 0,\ m > m' = 0,\ m = m' > 0$, and $m > m' > 0$. Note that the first term is zero for $E^{(a,b)}_{r,s}(\tau)$. We only prove the identity involving $E^{(1,1)}_{r,s}(\tau)$. In this case, we obtain

$$E^{(1,1)}_{r,s}(\tau) = \frac{1}{(2\pi\sqrt{-1})^{r+s}}\Bigg(\sum_{\substack{m=m'>0\\ n>n'\\ m,m'\equiv 1}} + \sum_{\substack{m>m'>0\\ m,m'\equiv 1\in\mathbb{Z}}}\Bigg)\frac{1}{(m\tau+n)^r(m'\tau+n')^s}.$$

The second term is easily seen to be

$$\sum_{\substack{m>m'>0\\ m,m'\equiv 1}} \varphi_r(q^m)\varphi_s(q^{m'}).$$

For the calculation of the first term, we need the partial fraction decomposition

$$\begin{aligned}\frac{1}{(\tau+n)^r(\tau+n')^s} =&(-1)^s\sum_{i=0}^{r-1}\binom{s+i-1}{i}\frac{1}{(\tau+n)^{r-i}}\cdot\frac{1}{(n-n')^{s+i}}\\ &+\sum_{j=0}^{s-1}(-1)^j\binom{r+j-1}{j}\frac{1}{(\tau+n')^{s-j}}\cdot\frac{1}{(n-n')^{r+j}}.\end{aligned} \tag{4.27}$$

Let $h = n - n'$. Then h is a positive integer. Using (4.27), the first term can be calculated as

$$\begin{aligned}&\frac{1}{(2\pi\sqrt{-1})^{r+s}}\sum_{\substack{m=m'>0\\ n>n'\\ m,m'\equiv 1}}\frac{1}{(m\tau+n)^r(m'\tau+n')^s}\\ =&\frac{1}{(2\pi\sqrt{-1})^{r+s}}\sum_{m>0:\mathrm{odd}}\sum_{\substack{n>n'\\ n,n'\in\mathbb{Z}}}\frac{1}{(m\tau+n)^r(m\tau+n')^s}\\ =&\frac{1}{(2\pi\sqrt{-1})^{r+s}}\sum_{m>0:\mathrm{odd}}\sum_{\substack{n\in\mathbb{Z}\\ h\in\mathbb{Z}_{>0}}}\Bigg\{(-1)^s\sum_{i=0}^{r-1}\binom{s+i-1}{i}\frac{1}{(m\tau+n)^{r-i}}\frac{1}{h^{s+i}}\\ &+\sum_{j=0}^{s-1}(-1)^j\binom{r+j-1}{j}\frac{1}{(m\tau+n-h)^{s-j}}\frac{1}{h^{r+j}}\Bigg\}\end{aligned}$$

$$
\begin{aligned}
=&(-1)^s\sum_{i=0}^{r-1}\binom{s+i-1}{i}\sum_{h\in\mathbb{Z}_{>0}}\frac{(2\pi\sqrt{-1})^{-s-i}}{h^{s+i}}\sum_{m>0:\mathrm{odd}}\sum_{n\in\mathbb{Z}}\frac{(2\pi\sqrt{-1})^{-r+i}}{(m\tau+n)^{r-i}}\\
&+\sum_{j=0}^{s-1}(-1)^j\binom{r+j-1}{j}\sum_{h\in\mathbb{Z}_{>0}}\frac{(2\pi\sqrt{-1})^{-r-j}}{h^{r+j}}\sum_{m>0:\mathrm{odd}}\sum_{n\in\mathbb{Z}}\frac{(2\pi\sqrt{-1})^{-s+j}}{(m\tau+n-h)^{s-j}}\\
=&(-1)^s\sum_{i=0}^{r-2}\binom{s+i-1}{i}\widetilde{\zeta}(s+i)\sum_{m>0:\mathrm{odd}}\varphi_{r-i}(q^m)\\
&+\sum_{j=0}^{s-2}(-1)^j\binom{r+j-1}{j}\widetilde{\zeta}(r+j)\sum_{m>0:\mathrm{odd}}\varphi_{s-j}(q^m)\\
=&\sum_{\substack{p+h=r+s\\ p,h\geq 1}}\left\{(-1)^s\binom{p-1}{s-1}+(-1)^{p+r}\binom{p-1}{r-1}\right\}\widetilde{\zeta}(p)\sum_{m>0:\mathrm{odd}}\varphi_h(q^m).
\end{aligned}
$$

The cancellation of the terms for $i=r-1$ and $j=s-1$ in the third equality can be justified by computing Cauchy principal values. The final equality is obtained by setting $s+i=p, r-i=h$ in the first term and $r+j=p, s-j=h$ in the second. This completes the proof for $E^{(1,1)}_{r,s}(\tau)$, the verification of the other cases being left to the reader. $\square$

For an integer $k>0$, we define

$$
\begin{aligned}
E_k^{(0)}(q)&=2^kG_k^{(0)}(q^2)=\frac{(-1)^k}{(k-1)!}\sum_{n>0}\sigma_{k-1}(n)q^{2n},\\
E_k^{(1)}(q)&=2^k\big(G_k^{(0)}(q)-G_k^{(0)}(q^2)\big)=\frac{(-1)^k}{(k-1)!}\sum_{n>0}\Big(\sum_{\substack{d|n\\ n/d:\mathrm{odd}}}d^{k-1}\Big)q^n.
\end{aligned}
$$

These q-series are modular forms on $\Gamma_0(2)$ when $k\geq 4$ is even. For integers $r>0$ and $s\geq 0$, we put

$$
f_r^{(a)}(q)=\sum_{\substack{m>0\\ m\equiv a}}\varphi_r(q^m),\ \overline{f}_s^{(a)}(q)=-\sum_{\substack{m>0\\ m\equiv a}}m\varphi_{s+1}(q^m).
$$

Then one can write for $k\geq 1$

$$
E_k^{(1)}(q)=f_k^{(1)}(q), E_k^{(0)}(q)=\widetilde{\zeta}(k)+f_k^{(0)}(q), E_k^{(1)}(q)'=k\overline{f}_k^{(1)}(q), E_k^{(0)}(q)'=k\overline{f}_k^{(0)}(q),
$$

where $'$ means $q \cdot d/dq$, and set

$$\begin{aligned}
\vartheta^{(0,1)}_{r,s}(q) &= \delta_{r,2}\overline{f}^{(1)}_{s}(q) - \delta_{r,1}\overline{f}^{(1)}_{s-1}(q) + \delta_{s,1}\overline{f}^{(0)}_{r-1}(q) + \delta_{r,1}\delta_{s,1}\alpha_1,\\
\vartheta^{(1,0)}_{r,s}(q) &= \delta_{r,2}\overline{f}^{(0)}_{s}(q) - \delta_{r,1}\overline{f}^{(0)}_{s-1}(q) + \delta_{s,1}\overline{f}^{(1)}_{r-1}(q) + \delta_{r,1}\delta_{s,1}\alpha_2,\\
\vartheta^{(1,1)}_{r,s}(q) &= \delta_{r,2}\overline{f}^{(1)}_{s}(q) - \delta_{r,1}\overline{f}^{(1)}_{s-1}(q) + \delta_{s,1}(\overline{f}^{(1)}_{r-1}(q) + 2f^{(1)}_{r}(q)) + \delta_{r,1}\delta_{s,1}\alpha_3,
\end{aligned}$$

where $\alpha_1 = -\alpha_2 = \overline{f}^{(1)}_{0}(q)$ and $\alpha_3 = 2\overline{f}^{(1)}_{0}(q) + \overline{f}^{(0)}_{0}(q)$.

Definition 4.12. *For positive integers r and s, we define the regularized double Eisenstein series $E^{(a,b)}_{r,s}(q)$ by*

$$\begin{aligned}
E^{(0,1)}_{r,s}(q) &= \sum_{\substack{m>m'>0\\ m\equiv 0, m'\equiv 1}} \varphi_r(q^m)\varphi_s(q^{m'}) + \frac{1}{4}\vartheta^{(0,1)}_{r,s}(q),\\
E^{(1,0)}_{r,s}(q) &= \sum_{\substack{m>m'>0\\ m\equiv 1, m'\equiv 0}} \varphi_r(q^m)\varphi_s(q^{m'}) + \widetilde{\zeta}(s)f^{(1)}_{r}(q) + \frac{1}{4}\vartheta^{(1,0)}_{r,s}(q),\\
E^{(1,1)}_{r,s}(q) &= \sum_{\substack{m>m'>0\\ m, m'\equiv 1}} \varphi_r(q^m)\varphi_s(q^{m'})\\
&\quad + \sum_{\substack{p+h=r+s\\ p,h\geq 1}} \left((-1)^s\binom{p-1}{s-1} + (-1)^{p+r}\binom{p-1}{r-1}\right)\widetilde{\zeta}(p)f^{(1)}_{h}(q) + \frac{1}{4}\vartheta^{(1,1)}_{r,s}(q).
\end{aligned}$$

We now present the regularized double shuffle relation of the double Eisenstein series for the cusp 0. For positive integers r and s, we put

$$\mathcal{P}^{(a,b)}_{r,s}(q) = E^{(a)}_{r}(q)E^{(b)}_{s}(q) + \frac{1}{4}(\delta_{r,2}\overline{f}^{(b)}_{s}(q) + \delta_{s,2}\overline{f}^{(a)}_{r}(q)).$$

It can be shown that $\mathcal{P}^{(a,b)}_{r,s}(q)$ are modular forms on $\Gamma_0(2)$ when both r and s are even greater than 1.

Theorem 4.13. *For positive even integer k and integers $r, s \geq 1$ with $(r,s) \neq (1,1)$, we have*

$$\mathcal{P}^{(a,b)}_{r,s}(q) = E^{(a,b)}_{r,s}(q) + E^{(b,a)}_{s,r}(q) + \delta_{a,b}E^{(a)}_{r+s}(q) \tag{4.28}$$

$$= \sum_{\substack{i+j=k\\ i,j\geq 1}} \binom{i-1}{r-1} E^{(a+b,b)}_{i,j}(q) + \sum_{\substack{i+j=k\\ i,j\geq 1}} \binom{i-1}{s-1} E^{(a+b,a)}_{i,j}(q). \tag{4.29}$$

Proof. The proof will be divided into two steps. We first prove the equalities of the imaginary parts in Theorem 4.13. The only imaginary parts that appear come from the constant terms $\widetilde{\zeta}(s)$ of $E_s^{(0)}(q)$ (s : odd), $\widetilde{\zeta}(s)$ in $E_{r,s}^{(1,0)}(q)$ (s : odd) or $\widetilde{\zeta}(p)$ (p : odd) in $E_{r,s}^{(1,1)}(q)$. We consider the generating functions as follows:

$$\begin{aligned}
E_k^{(1,1)}(X,Y) &:= \sum_{\substack{r+s=k\\ r,s\geq 1}} \mathrm{Im}\ E_{r,s}^{(1,1)}(q) X^{r-1}Y^{s-1} \\
&= \sum_{\substack{r+s=k\\ r,s\geq 1}} \sum_{\substack{p+h=k\\ p,h\geq 1\\ p:\mathrm{odd}}} \left((-1)^s \binom{p-1}{s-1} + (-1)^{p+r} \binom{p-1}{r-1} \right) \widetilde{\zeta}(p) f_h^{(1)}(q) X^{r-1}Y^{s-1} \\
&= \sum_{\substack{p+h=k\\ p,h\geq 1\\ p:\mathrm{odd}}} (Y^{h-1}-X^{h-1})(Y-X)^{p-1}\widetilde{\zeta}(p) f_h^{(1)}(q), \\
E_k^{(1,0)}(X,Y) &:= \sum_{\substack{r+s=k\\ r,s\geq 1}} \mathrm{Im}\ E_{r,s}^{(1,0)}(q) X^{r-1}Y^{s-1} = \sum_{\substack{r+s=k\\ r,s\geq 1\\ s:\mathrm{odd}}} \widetilde{\zeta}(s) f_r^{(1)}(q) X^{r-1}Y^{s-1}.
\end{aligned}$$

When $(a,b)=(1,0)$, we note that the imaginary part of the R.H.S. of (4.29) is the coefficient of $X^{r-1}Y^{s-1}$ of $E_k^{(1,0)}(X+Y,Y)+E_k^{(1,1)}(X+Y,X)$. Since we have

$$\begin{aligned}
& E_k^{(1,0)}(X+Y,Y)+E_k^{(1,1)}(X+Y,X) \\
&= \sum_{\substack{r+s=k\\ r,s\geq 1\\ s:\mathrm{odd}}} \widetilde{\zeta}(s) f_r^{(1)}(q)(X+Y)^{r-1}Y^{s-1} + \sum_{\substack{r+s=k\\ r,s\geq 1\\ s:\mathrm{odd}}} (X^{r-1}-(X+Y)^{r-1})(-Y)^{s-1}\widetilde{\zeta}(s) f_r^{(1)}(q) \\
&= \sum_{\substack{r+s=k\\ r,s\geq 1\\ s:\mathrm{odd}}} \left((X+Y)^{r-1}Y^{s-1} + (X^{r-1}-(X+Y)^{r-1})Y^{s-1}\right) \widetilde{\zeta}(s) f_r^{(1)}(q) \\
&= \sum_{\substack{r+s=k\\ r,s\geq 1\\ s:\mathrm{odd}}} \widetilde{\zeta}(s) f_r^{(1)}(q) X^{r-1}Y^{s-1},
\end{aligned}$$

the assertion follows. Secondly, we prove the equalities of the real parts in Theorem 4.13. Again we use generating functions. Define

$$f_{r,s}^{(a,b)}(q) = \sum_{\substack{m>m'>0\\ m\equiv 0, m'\equiv 1}} \varphi_r(q^m)\varphi_s(q^{m'}),$$

$$\gamma_{r,s}(q) = \sum_{\substack{p+h=r+s\\ p,h\geq 1}} \left((-1)^s\binom{p-1}{s-1} + (-1)^{p+r}\binom{p-1}{r-1}\right)\beta_p f_h^{(1)}(q),$$

where $\beta_p = -B_p/2p!(=\widetilde{\zeta}(p), p : \text{even})$. Consider

$$\begin{aligned}
E^{(1)}(X) &:= \sum_{r\geq 1} E_r^{(1)}(q)X^{r-1} - \frac{\alpha_3}{2}\cdot X,\ E^{(a,b)}(X,Y) := \sum_{r,s\geq 1} \text{Re } E_{r,s}^{(a,b)}(q)X^{r-1}Y^{s-1},\\
\gamma(X,Y) &:= \sum_{r,s\geq 1} \gamma_{r,s}(q)X^{r-1}Y^{s-1},\ \mathcal{P}^{(a,b)}(X,Y) := \sum_{r,s\geq 1} \text{Re } \mathcal{P}_{r,s}^{(a,b)}(q)X^{r-1}Y^{s-1}.
\end{aligned} \tag{4.30}$$

Then, it is sufficient to prove that

$$\mathcal{P}^{(a,b)}(X,Y) = E^{(a,b)}(X,Y) + E^{(b,a)}(Y,X) + \delta_{(a,b),(1,1)}\frac{E^{(1)}(X) - E^{(1)}(Y)}{X-Y} \tag{4.31}$$

$$= E^{(a+b,b)}(X+Y,Y) + E^{(a+b,a)}(X+Y,X). \tag{4.32}$$

Now we check the equalities in (4.31) and (4.32). Write $a(X)$ and $a(X,Y)$ for the generating functions $\sum_{k\geq 1} a_k X^{k-1}$ and $\sum_{r,s\geq 1} a_{r,s}X^{r-1}Y^{s-1}$ associated with sequences $\{a_k\}$ and $\{a_{r,s}\}$ indexed by one and two integers, respectively. Then we have

$$\begin{aligned}
\beta(X) &= \sum_{k\geq 1} \beta_k X^{k-1} = \frac{1}{2}\left(\frac{1}{X} - \frac{1}{e^X - 1}\right),\\
f^{(1)}(X) &= \sum_{k\geq 1} f_k^{(1)}(q)X^{k-1} = -\sum_{u>0} e^{-uX}\frac{q^u}{1-q^{2u}},\\
f^{(0)}(X) &= \sum_{k\geq 1} f_k^{(0)}(q)X^{k-1} = -\sum_{u>0} e^{-uX}\frac{q^{2u}}{1-q^{2u}},\\
\overline{f}^{(1)}(X) &= \sum_{k\geq 1} \overline{f}_k^{(1)}(q)X^{k-1} = \frac{1}{X}\left(\sum_{u>0} e^{-uX}\frac{2q^u}{(1-q^{2u})^2} + f^{(1)}(X) - \overline{f}_0^{\mathbf{o}}(q)\right),\\
\overline{f}^{(0)}(X) &= \sum_{k\geq 1} \overline{f}_k^{(0)}(q)X^{k-1} = \frac{1}{X}\left(\sum_{u>0} e^{-uX}\frac{2q^{2u}}{(1-q^{2u})^2} - \overline{f}_0^{(0)}(q)\right),
\end{aligned}$$

$$
\begin{aligned}
f^{(0,1)}(X,Y) &= \sum_{r,s\geq 1} f^{(0,1)}_{r,s}(q) X^{r-1}Y^{s-1} = \sum_{u,v>0} e^{-uX-vY} \sum_{\substack{m>m'>0\\ m\equiv 0, m'\equiv 1}} q^{um+vm'} \\
&= \sum_{u,v>0} e^{-uX-vY} \frac{q^u}{1-q^{2u}} \frac{q^{u+v}}{1-q^{2(u+v)}}, \\
f^{(1,0)}(X,Y) &= \sum_{r,s\geq 1} f^{(1,0)}_{r,s}(q) X^{r-1}Y^{s-1} = \sum_{u,v>0} e^{-uX-vY} \frac{q^u}{1-q^{2u}} \frac{q^{2(u+v)}}{1-q^{2(u+v)}}, \\
f^{(1,1)}(X,Y) &= \sum_{r,s\geq 1} f^{(1,1)}_{r,s}(q) X^{r-1}Y^{s-1} = \sum_{u,v>0} e^{-uX-vY} \frac{q^{2u}}{1-q^{2u}} \frac{q^{u+v}}{1-q^{2(u+v)}}, \\
\vartheta^{(0,1)}(X,Y) &= X\overline{f}^{(1)}(Y) - Y\overline{f}^{(1)}(Y) - \overline{f}^{(1)}_0(q) + X\overline{f}^{(0)}(X) + \overline{f}^{(0)}_0(q) + \alpha_1, \\
\vartheta^{(1,0)}(X,Y) &= X\overline{f}^{(0)}(Y) - Y\overline{f}^{(0)}(Y) - \overline{f}^{(0)}_0(q) + X\overline{f}^{(1)}(X) + \overline{f}^{(1)}_0(q) + \alpha_2, \\
\vartheta^{(1,1)}(X,Y) &= X\overline{f}^{(1)}(Y) - Y\overline{f}^{(1)}(Y) + X\overline{f}^{(1)}(X) + 2f^{(1)}(X) + \alpha_3.
\end{aligned}
$$

By the definitions (4.30), we find

$$
\begin{aligned}
E^{(1)}(X) &= f^{(1)}(X) - \frac{\alpha_3}{2}\cdot X, \\
E^{(0,1)}(X,Y) &= f^{(0,1)}(X,Y) + \frac{1}{4}\vartheta^{(0,1)}(X,Y), \\
E^{(1,0)}(X,Y) &= f^{(1,0)}(X,Y) + f^{(1)}(X)\beta(Y) + \frac{1}{4}\vartheta^{(1,0)}(X,Y), \\
E^{(1,1)}(X,Y) &= f^{(1,1)}(X,Y) + \gamma(X,Y) + \frac{1}{4}\vartheta^{(1,1)}(X,Y), \\
\mathcal{P}^{(1,0)}(X,Y) &= f^{(1)}(X)f^{(0)}(Y) + f^{(1)}(X)\beta(Y) + \frac{1}{4}\big(X\overline{f}^{(0)}(Y) + Y\overline{f}^{(1)}(X)\big), \\
\mathcal{P}^{(1,1)}(X,Y) &= f^{(1)}(X)f^{(1)}(Y) + \frac{1}{4}\big(X\overline{f}^{(1)}(Y) + Y\overline{f}^{(1)}(X)\big).
\end{aligned}
$$

For the right-hand side of (4.31) with $(a,b)=(1,1)$, we compute

$$
\begin{aligned}
&f^{(1,1)}(X,Y)+f^{(1,1)}(Y,X)\\
&=\sum_{u,v>0}e^{-uX-vY}\left(\frac{q^{2u}}{1-q^{2u}}+\frac{q^{2v}}{1-q^{2v}}\right)\frac{q^{u+v}}{1-q^{2(u+v)}}\\
&=\sum_{u,v>0}e^{-uX-vY}\left(\frac{q^{u}}{1-q^{2u}}\frac{q^{v}}{1-q^{2v}}-\frac{q^{u+v}}{1-q^{2(u+v)}}\right)\\
&=f^{(1)}(X)f^{(1)}(Y)-\sum_{w>u>0}e^{-(w-u)Y-uX}\frac{q^{w}}{1-q^{2w}}\quad(w=u+v)\\
&=f^{(1)}(X)f^{(1)}(Y)-\sum_{w>0}\frac{q^{w}}{1-q^{2w}}e^{-wY}\left(e^{Y-X}\frac{1-e^{(Y-X)(w-1)}}{1-e^{Y-X}}\right)\\
&=f^{(1)}(X)f^{(1)}(Y)+\frac{e^{Y}}{e^{X}-e^{Y}}f^{(1)}(Y)-\frac{e^{X}}{e^{X}-e^{Y}}f^{(1)}(X)\\
&=f^{(1)}(X)f^{(1)}(Y)-\frac{1}{2}(f^{(1)}(X)+f^{(1)}(Y))-\frac{1}{2}\coth\left(\frac{X-Y}{2}\right)(f^{(1)}(X)-f^{(1)}(Y)),\\
&\gamma(X,Y)+\gamma(Y,X)\\
&=(\beta(Y-X)-\beta(X-Y))(f^{(1)}(X)-f^{(1)}(Y))\\
&=-\frac{f^{(1)}(X)-f^{(1)}(Y)}{X-Y}+\frac{1}{2}\coth\left(\frac{X-Y}{2}\right)(f^{(1)}(X)-f^{(1)}(Y)),\\
&\vartheta^{(1,1)}(X,Y)+\vartheta^{(1,1)}(Y,X)\\
&=X\overline{f}^{(1)}(Y)+Y\overline{f}^{(1)}(X)+2f^{(1)}(X)+2f^{(1)}(Y)+2\alpha_3.
\end{aligned}
$$

Combining these with $(E^{(1)}(X)-E^{(1)}(Y))/(X-Y)$, we have

$$
\begin{aligned}
&E^{(1,1)}(X,Y)+E^{(1,1)}(Y,X)+\frac{E^{(1)}(X)-E^{(1)}(Y)}{X-Y}\\
&=f^{(1)}(X)f^{(1)}(Y)-\frac{1}{2}(f^{(1)}(X)+f^{(1)}(Y))-\frac{1}{2}\coth\left(\frac{X-Y}{2}\right)(f^{(1)}(X)-f^{(1)}(Y))\\
&-\frac{f^{(1)}(X)-f^{(1)}(Y)}{X-Y}+\frac{1}{2}\coth\left(\frac{X-Y}{2}\right)(f^{(1)}(X)-f^{(1)}(Y))\\
&+\frac{1}{4}\left(X\overline{f}^{(1)}(Y)+Y\overline{f}^{(1)}(X)+2f^{(1)}(X)+2f^{(1)}(Y)+2\alpha_3\right)+\frac{f^{(1)}(X)-f^{(1)}(Y)}{X-Y}-\frac{\alpha_3}{2}\\
&=f^{(1)}(X)f^{(1)}(Y)+\frac{1}{4}(X\overline{f}^{(1)}(Y)+Y\overline{f}^{(1)}(X)).
\end{aligned}
$$

For the right-hand side of (4.32) with $(a,b)=(1,1)$, we proceed as follows:

$$\begin{aligned}
&f^{(0,1)}(X+Y,X)+f^{(0,1)}(X+Y,Y)\\
&=\sum_{u,v>0}\left(e^{-(u+v)X-uY}+e^{-uX-(u+v)Y}\right)\frac{q^u}{1-q^{2u}}\frac{q^{u+v}}{1-q^{2(u+v)}}\\
&=\left(\sum_{w>u>0}+\sum_{u>w>0}\right)e^{-uX-wY}\frac{q^u}{1-q^{2u}}\frac{q^w}{1-q^{2w}}\\
&=\left(\sum_{w,u>0}-\sum_{w=u>0}\right)e^{-uX-wY}\frac{q^u}{1-q^{2u}}\frac{q^w}{1-q^{2w}}\\
&=f^{(1)}(X)f^{(1)}(Y)-\sum_{u>0}e^{-u(X+Y)}\frac{q^{2u}}{(1-q^{2u})^2}\\
&=f^{(1)}(X)f^{(1)}(Y)-\frac{1}{2}\overline{f}_0^{(0)}(q)-\frac{1}{2}(X+Y)\overline{f}^{(0)}(X+Y),\\
&\vartheta^{(0,1)}(X+Y,X)+\vartheta^{(0,1)}(X+Y,Y)\\
&=Y\overline{f}^{(1)}(X)+X\overline{f}^{(1)}(Y)+2(X+Y)\overline{f}^{(0)}(X+Y)+2(\alpha_1-\overline{f}_0^{(1)}(q)+\overline{f}_0^{(0)}(q)).
\end{aligned}$$

Summing these up, we have

$$\begin{aligned}
&E^{(0,1)}(X+Y,Y)+E^{(0,1)}(X+Y,X)\\
&=f^{(1)}(X)f^{(1)}(Y)-\frac{1}{2}\overline{f}_0^{(0)}(q)-\frac{1}{2}(X+Y)\overline{f}^{(0)}(X+Y)\\
&+\frac{1}{4}\left(Y\overline{f}^{(1)}(X)+X\overline{f}^{(1)}(Y)+2(X+Y)\overline{f}^{(0)}(X+Y)+2(\alpha_1-\overline{f}_0^{(1)}(q)+\overline{f}_0^{(0)}(q))\right)\\
&=f^{(1)}(X)f^{(1)}(Y)+\frac{1}{4}(X\overline{f}^{(1)}(Y)+Y\overline{f}^{(1)}(X)).
\end{aligned}$$

For the right-hand side of (4.31) with $(a,b)=(1,0)$, we compute

$$\begin{aligned}
&f^{(1,0)}(X,Y)+f^{(0,1)}(Y,X)\\
&=\sum_{u,v>0}e^{-uX-vY}\left(\frac{q^v}{1-q^{2v}}+\frac{q^{2u+v}}{1-q^{2u}}\right)\frac{q^{u+v}}{1-q^{2(u+v)}}\\
&=\sum_{u,v>0}e^{-uX-vY}\frac{q^u}{1-q^{2u}}\frac{q^{2v}}{1-q^{2v}}=f^{(1)}(X)f^{(0)}(Y),\\
&\vartheta^{(1,0)}(X,Y)+\vartheta^{(0,1)}(Y,X)=X\overline{f}^{(0)}(Y)+Y\overline{f}^{(1)}(X)+\alpha_1+\alpha_2,
\end{aligned}$$

to obtain

$$E^{(1,0)}(X,Y)+E^{(0,1)}(Y,X)=f^{(1)}(X)f^{(0)}(Y)+f^{(1)}(X)\beta(Y)+\frac{1}{4}(X\overline{f}^{(0)}(Y)+Y\overline{f}^{(1)}(X)).$$

Finally, for the right-hand side of (4.32) with $(a,b)=(1,0)$, we similarly compute

$$\begin{aligned}
&f^{(1,0)}(X+Y,Y)+f^{(1,1)}(X+Y,X)\\
&=\left(\sum_{w>u>0}+\sum_{u>w>0}\right)e^{-uX-vY}\frac{q^u}{1-q^{2u}}\frac{q^{2w}}{1-q^{2w}}\\
&=\left(\sum_{w,u>0}-\sum_{u=w>0}\right)e^{-uX-vY}\frac{q^u}{1-q^{2u}}\frac{q^{2w}}{1-q^{2w}}\\
&=f^{(1)}(X)f^{(0)}(Y)-\sum_{u>0}e^{-u(X+Y)}\frac{q^{3u}}{(1-q^{2u})^2}\\
&=f^{(1)}(X)f^{(0)}(Y)-\sum_{u>0}e^{-u(X+Y)}\left(\frac{q^u}{(1-q^{2u})^2}-\frac{q^u}{1-q^{2u}}\right)\\
&=f^{(1)}(X)f^{(0)}(Y)-\frac{1}{2}\left((X+Y)\overline{f}^{(1)}(X+Y)-f^{(1)}(X+Y)+\overline{f}_0^{(1)}(q)\right)-f^{(1)}(X+Y)\\
&=f^{(1)}(X)f^{(0)}(Y)-\frac{1}{2}f^{(1)}(X+Y)-\frac{1}{2}(X+Y)\overline{f}^{(1)}(X+Y)-\frac{1}{2}\overline{f}_0^{(1)}(q),\\
&f^{(1)}(X+Y)\beta(Y)+\gamma(X+Y,X)=f^{(1)}(X)\beta(Y),\\
&\vartheta^{(1,0)}(X+Y,Y)+\vartheta^{(1,1)}(X+Y,X)\\
&=X\overline{f}^{(0)}(Y)+Y\overline{f}^{(1)}(X)+2(X+Y)\overline{f}^{(1)}(X+Y)+2f^{(1)}(X+Y)-\overline{f}_0^{(0)}(q)+\overline{f}_0^{(1)}(q)+\alpha_3+\alpha_2,
\end{aligned}$$

which give

$$\begin{aligned}
&E^{(1,0)}(X+Y,Y)+E^{(1,1)}(X+Y,X)\\
&=f^{(1)}(X)f^{(0)}(Y)-\frac{1}{2}f^{(1)}(X+Y)-\frac{1}{2}(X+Y)\overline{f}^{(1)}(X+Y)-\frac{1}{2}\overline{f}_0^{(1)}(q)+f^{(1)}(X)\beta(Y)+\\
&\frac{1}{4}\left(X\overline{f}^{(0)}(Y)+Y\overline{f}^{(1)}(X)+2(X+Y)\overline{f}^{(1)}(X+Y)+2f^{(1)}(X+Y)-\overline{f}_0^{(0)}(q)+\overline{f}_0^{(1)}(q)+\alpha_3+\alpha_2\right)\\
&=f^{(1)}(X)f^{(0)}(Y)+f^{(1)}(X)\beta(Y)+\frac{1}{4}(X\overline{f}^{(0)}(Y)+Y\overline{f}^{(1)}(X)),
\end{aligned}$$

and we are done. $\square$

As an analogue of Theorem 4.6, we have the following:

Theorem 4.14. *Let $k\geq 4$ be a positive even integer and set $\mathcal{DE}_k^{(0)}=\langle E_{2i,k-2i}^{(1,1)}(q)\mid$*

$1 \leq i \leq k/2-1\big\rangle_{\mathbb{Q}}$.
(i) Then the space $\mathcal{DE}_k^{(0)}$ *contains* $\mathbb{Q}\cdot E_k^{(1)}(q)\oplus S_k^{\mathbb{Q}}(2)$.
(ii)

$$\dim \mathcal{DE}_k^{(0)} = \frac{k}{2}-1,$$

so that the series $E_{r,k-r}^{(1,1)}(q)$ *(*r *even) are linearly independent over* $\mathbb{Q}$.

5 More on $\varepsilon_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$

5.1 Period polynomial for $\Gamma_0(2)$

We fix and recall the notations as follows.

- $\Gamma_0(2)=\{\left(\begin{smallmatrix} a & b \\ c & d\end{smallmatrix}\right)\in\Gamma_1 \mid c\equiv 0 \pmod 2\}$
- $S_k(2)$: the $\mathbb{C}$-vector space spanned by cusp forms of weight k for $\Gamma_0(2)$
- $V_{k,2}=\langle x_1^{s_1-1}x_2^{s_2-1} \mid (s_1,s_2)\in S_{k,2}\rangle_{\mathbb{Q}}$
- $W_{k,2}^{-,0}=\big\{p(x_1,x_2)\in V_{k,2} \mid p(x_1,x_2)=p(x_2-x_1,x_2)-p(x_2-x_1,x_2-2x_1)+p(x_1,x_2-2x_1)\big\}$: the $\mathbb{Q}$-vector space generated by restricted even period polynomials for $\Gamma_0(2)$
- $T_{k,2}=\{(k_1,k_2)\in\mathbb{Z}_{\geq 2}^2 \mid k_1+k_2=k,\ k_i:\text{even}\}$
- $\mathcal{A}_{k,2}$: the $|S_{k,2}|\times|T_{k,2}|$ matrix whose entries are the integer $\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}$, so that

$$\mathcal{A}_{k,2}=\Big(\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}\Big)_{\substack{(s_1,s_2)\in S_{k,2}\\ (k_1,k_2)\in T_{k,2}}}.$$

In [9], we obtain a characterization of the left kernel of $\mathcal{A}_{k,2}$, which is an analogous result to Proposition 2.1.

Theorem 5.1. *Let* $(a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}}$ *be a vector with rational coefficients. Then the following assertions are equivalent.*
(i) The vector $(a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}}$ *is a left annihilator of the matrix* $\mathcal{A}_{k,2}$.
(ii) The polynomial $\sum_{(s_1,s_2)\in S_{k,2}} a_{s_2,s_1}x_1^{s_1-1}x_2^{s_2-1}$ *is an element of the space* $W_{k,2}^{-,0}$.

Proof. Assume that $(a_{s_1,s_2})_{(s_1,s_2)\in S_{k,2}}$ is a left annihilator of $\mathcal{A}_{k,2}$. Set the polynomial $p(x_1,x_2)=\sum_{(s_1,s_2)\in S_{k,2}} a_{s_2,s_1}x_1^{s_1-1}x_2^{s_2-1}$. Then we can compute

$$
\begin{aligned}
0 &= \sum_{(k_1,k_2)\in T_{k,2}} \Big(\sum_{(s_1,s_2)\in S_{k,2}} \varepsilon_{\binom{s_2,s_1}{k_1,k_2}} a_{s_2,s_1} \Big) x_1^{k_1-1}x_2^{k_2-1} \\
&= \sum_{(s_1,s_2)\in S_{k,2}} a_{s_2,s_1} \sum_{(k_1,k_2)\in T_{k,2}} C^{s_2}_{k_1,k_2} x_1^{k_1-1}x_2^{k_2-1} \\
&= \frac{1}{2}\Big(p(x_1,x_2-x_1) - p(x_2,x_2-x_1) - p(x_1,x_1+x_2) + p(x_2,x_1+x_2) \Big).
\end{aligned}
$$

Letting $x_2 \mapsto x_2 - x_1$, we have

$$
0 = p(x_1,x_2) - p(x_2-x_1,x_2) - p(x_1,x_2-2x_1) + p(x_2-x_1,x_1-2x_1),
$$

which means $p(x_1,x_2)\in W^{-,0}_{k,2}$. For the polynomial $f(x_1,x_2)$ satisfying $f(x_1,0)=0$, it can be shown that $f(x_1,x_2-x_1)$ is 0 if and only if $f(x_1,x_2)=0$. This implies the assertion (ii)⇒(i). $\square$

Theorem 5.1 has an application to determine the dimension of the space $W^{-,0}_{k,2}$. We now discuss the rank of the matrix $\mathcal{A}_{k,2}$ to prove $\dim W^{-,0}_{k,2} = \dim S_k(2)$. By definition, for each $(s_1,s_2)\in S_{k,2}$ and $(k_1,k_2)\in T_{k,2}$, $\varepsilon_{\binom{s_1,s_2}{k_1,k_2}}$ is zero if $s_1<\min\{k_1,k_2\}$ or $k_1=k_2$. Since $\varepsilon_{\binom{s_1,s_2}{k_1,k_2}} = -\varepsilon_{\binom{s_1,s_2}{k_2,k_1}}$, the matrix $\mathcal{A}_{k,2}$ can be reduced to the forms

$$
\begin{pmatrix}
\varepsilon_{\binom{3,k-3}{2,k-2}} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
\varepsilon_{\binom{5,k-5}{2,k-2}} & \varepsilon_{\binom{5,k-5}{4,k-4}} & 0 & \cdots & 0 & 0 & \cdots & 0 \\
\varepsilon_{\binom{7,k-7}{2,k-2}} & \varepsilon_{\binom{7,k-7}{4,k-4}} & \varepsilon_{\binom{7,k-7}{6,k-6}} & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\varepsilon_{\binom{k/2-1,k/2+1}{2,k-2}} & \varepsilon_{\binom{k/2-1,k/2+1}{4,k-4}} & \varepsilon_{\binom{k/2-1,k/2+1}{6,k-6}} & \cdots & \varepsilon_{\binom{k/2-1,k/2+1}{k/2-2,k/2+2}} & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\varepsilon_{\binom{k-3,3}{2,k-2}} & \varepsilon_{\binom{k-3,3}{4,k-4}} & \varepsilon_{\binom{k-3,3}{6,k-6}} & \cdots & \varepsilon_{\binom{k-3,3}{k/2-2,k/2+2}} & 0 & \cdots & 0
\end{pmatrix}
$$

if $k \equiv 0 \pmod 4$, and

$$\begin{pmatrix}
\mathcal{E}\binom{3,k-3}{2,k-2} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
\mathcal{E}\binom{5,k-5}{2,k-2} & \mathcal{E}\binom{5,k-5}{4,k-4} & 0 & \cdots & 0 & 0 & \cdots & 0 \\
\mathcal{E}\binom{7,k-7}{2,k-2} & \mathcal{E}\binom{7,k-7}{4,k-4} & \mathcal{E}\binom{7,k-7}{6,k-6} & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\mathcal{E}\binom{k/2-2,k/2+2}{2,k-2} & \mathcal{E}\binom{k/2-2,k/2+2}{4,k-4} & \mathcal{E}\binom{k/2-2,k/2+2}{6,k-6} & \cdots & \mathcal{E}\binom{k/2,k/2}{k/2-1,k/2+1} & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\mathcal{E}\binom{k-3,3}{2,k-2} & \mathcal{E}\binom{k-3,3}{4,k-4} & \mathcal{E}\binom{k-3,3}{6,k-6} & \cdots & \mathcal{E}\binom{k-3,3}{k/2-1,k/2+1} & 0 & \cdots & 0
\end{pmatrix}$$

if $k \equiv 2 \pmod 4$. Since all diagonal components are non-zeros, we have

$$\operatorname{rank} \mathcal{A}_{k,2} = \left[\frac{k+2}{4}\right] - 1. \tag{5.1}$$

This implies $\dim\ker \mathcal{A}_{k,2} = [k/4] - 1 = \dim S_k(2)$. Therefore, from Theorem 5.1 we have $\dim W_{k,2}^{-,0} = \dim S_k(2)$. As a corollary, we can obtain the Eichler-Shimura-Manin correspondence for $\Gamma_0(2)$.

Theorem 5.2. [9, Theorem 4] *For even k, there is an isomorphism*

$$r^{-,0} : S_k(2) \longrightarrow W_{k,2}^{-,0} \otimes_{\mathbb{Q}} \mathbb{C}.$$

Example. We give a few examples.

$$\mathcal{A}_{8,2} = \begin{pmatrix} 2 & 0 & -2 \\ 4 & 0 & -4 \end{pmatrix}, \ \mathcal{A}_{10,2} = \begin{pmatrix} 2 & 0 & 0 & -2 \\ 4 & 4 & -4 & -4 \\ 6 & 14 & -14 & -6 \end{pmatrix}, \ \mathcal{A}_{12,2} = \begin{pmatrix} 2 & 0 & 0 & 0 & -2 \\ 4 & 4 & 0 & -4 & -4 \\ 6 & 20 & 0 & -20 & -6 \\ 8 & 48 & 0 & -48 & -8 \end{pmatrix}.$$

Each of left kernels is spanned by the set $\{(-2,1)\}$, $\{(8,-7,2)\}$ and $\{(20,-12,0,1),(7,-5,1,0)\}$, respectively. We can easily find the correspondence with the following bases:

$$\begin{aligned}
W_{8,2}^{-,0} &= \mathbb{Q}\cdot(x_1^2x_2^4 - 2x_1^4x_2^2), \\
W_{10,2}^{-,0} &= \mathbb{Q}\cdot(2x_1^2x_2^6 - 7x_1^4x_2^4 + 8x_1^4x_2^6), \\
W_{12,2}^{-,0} &= \mathbb{Q}\cdot(x_1^2x_2^8 - 3x_1^4x_2^6 + 3x_1^6x_2^4 - x_1^8x_2^2) + \mathbb{Q}\cdot(x_1^4x_2^6 - 5x_1^6x_2^4 + 7x_1^8x_2^2).
\end{aligned}$$

Remark. We give an interesting observation for the level 2 version of the matrix $\mathcal{E}_{k,r}$: define

$$\mathcal{A}_{k,r}=\left(\varepsilon_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}\right)_{\substack{(s_1,\dots,s_r)\in S_{k,r}\\(k_1,\dots,k_r)\in T_{k,r}}},$$

where $T_{k,r}=\{(k_1\dots,k_r)\in\mathbb{Z}^r_{\geq 2}\mid k_1+\cdots+k_r=k,\ k_i:\text{odd }(1\leq i\leq r-2),\ k_{r-1},k_r:\text{even}\}$. Then, numerical computations show that for $r\geq 3$ the dimension of the left kernel of the matrix $\mathcal{A}_{k,r}$ is given by

$$\sum_{k>0}\dim\ker\mathcal{A}_{k,r}x^k\stackrel{?}{=}\mathbb{O}(x)^{r-2}\mathbb{S}_2(x),$$

where $\mathbb{S}_2(x)=\sum_{k>0}\dim S_k(2)x^k$. (I have checked this for $r\leq 5$ and $k\leq 30$.)

5.2 Almost totally odd MZVs

Denote by $\overline{\mathcal{Z}}_{k,r}$ the quotient vector space $\mathcal{Z}_k^{(r)}/\mathcal{Z}_k^{(r-1)}$, and $\zeta_{\mathfrak{D}}(\mathbf{k})$ the equivalence class of $\zeta(\mathbf{k})$ of weight k and depth r in $\overline{\mathcal{Z}}_{k,r}$. When $k_i\geq 3$ $(1\leq i\leq r-1)$ (odd) and $k_r\geq 2$ (even), we call $\zeta_{\mathfrak{D}}(k_1,\dots,k_r)$ the almost totally odd MZVs. Let $U_{k,r}$ be the set of almost totally odd indices of weight k and depth r:

$$U_{k,r}=\{(k_1,\dots,k_r)\in\mathbb{Z}^r_{\geq 2}\mid k_1+\cdots+k_r=k,\ k_r:\text{even},\ k_i:\text{odd }(1\leq i\leq r-1)\}.$$

We note that if $k\not\equiv r \pmod 2$, then $U_{k,r}$ is the empty set. Let us denote by $\mathcal{U}_{k,r}$ the $\mathbb{Q}$-vector subspace of $\overline{\mathcal{Z}}_{k,r}$ spanned by almost totally odd MZVs of weight k and depth r:

$$\mathcal{U}_{k,r}=\langle\zeta_{\mathfrak{D}}(\mathbf{k})\mid\mathbf{k}\in U_{k,r}\rangle_{\mathbb{Q}}.$$

The space $\mathcal{U}_{k,2}$ relates with both even and odd period polynomials on Γ_1, which was discovered by Zagier [15]. We define the space of odd period polynomials W_k^+ by

$$W_k^+=\left\{p(x_1,x_2)\in\bigoplus_{(k_1,k_2)\in T_{k,2}}\mathbb{Q}x_1^{k_1-1}x_2^{k_2-1}\;\middle|\;p(x_1,x_2)=p(x_2-x_1,x_2)+p(x_2-x_1,x_1)\right\}.$$

Note that, from the Eichler-Shimura-Manin correspondence, we have $\dim W_k^+=\dim S_k(\Gamma_1)$. Consider the $|U_{k,r}|\times|U_{k,r}|$ matrix

$$\mathcal{B}_{k,r}=\left(c_{\binom{s_1,\dots,s_r}{k_1,\dots,k_r}}\right)_{\substack{(s_1,\dots,s_r)\in U_{k,r}\\(k_1,\dots,k_r)\in U_{k,r}}},$$

where the integer $c_{\binom{s_1,\ldots,s_r}{k_1,\ldots,k_r}}$ is defined in (2.14).

Proposition 5.3. [15, Section 6] *For each odd integer $k > 0$, there is an injective map*

$$W_{k-1}^{+} \oplus W_{k+1}^{-,0} \longrightarrow \ker \mathcal{B}_{k,2}.$$

Since the right annihilator of $\mathcal{B}_{k,2}$ gives a linear relation among almost totally odd double zeta values, we obtain the following:

Theorem 5.4. [15, Theorem 3] *For each odd integer $k \geq 5$, we have*

$$\dim \mathcal{U}_{k,2} \leq |U_{k,2}| - \dim S_{k-1}(\Gamma_1) - \dim S_{k+1}(\Gamma_1).$$

In general, as in the case of the matrix $\mathcal{C}_{k,r}$, we may expect that any right annihilator $(a_{k_1,\ldots,k_r})_{(k_1,\ldots,k_r)\in U_{k,r}}$ of the matrix $\mathcal{B}_{k,r}$ gives a linear relation

$$\sum_{(k_1,\ldots,k_r)\in U_{k,r}} a_{k_1,\ldots,k_r} \zeta_{\mathfrak{d}}(k_1,\ldots,k_r) \stackrel{?}{=} 0,$$

and all linear relations among almost totally odd MZVs arise from the right kernel of the matrix $\mathcal{B}_{k,r}$. For this expectation, we present some numerical evidence as follows.

♣ Numerical dimension of $\mathcal{U}_{k,r}$.

$n\backslash k$	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	1		1		1		1		1		1		1		1		1		1
2				1		2		3		3		4		5		5		6	
3							1		3		5		8		11		15		19
4										1		4		9		16		-	
5													1		5		-		-

♣ Numerical rank of $\mathcal{B}_{k,r}$.

$n\backslash k$	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	1		1		1		1		1		1		1		1		1		1
2				1		2		3		3		4		5		5		6	
3							1		3		5		8		11		15		19
4										1		4		9		16		26	
5													1		5		14		29

We note that $\sum_{k>0}|U_{k,r}|x^k = \mathbb{E}(x)\mathbb{O}(x)^{r-1}$, where $\mathbb{E}(x) = \frac{x^2}{1-x^2}$. For $r \in \{2,3,4\}$, numerical computations suggest that the generating series of rank $\mathcal{B}_{k,r}$ is given by

$$\sum_{k>0} \text{rank } \mathcal{B}_{k,2}x^k \stackrel{?}{=} \mathbb{E}(x)\mathbb{O}(x) - (x+\frac{1}{x})\mathbb{S}(x),$$
$$\sum_{k>0} \text{rank } \mathcal{B}_{k,3}x^k \stackrel{?}{=} \mathbb{E}(x)\mathbb{O}(x)^2 - \frac{1}{x^2}\mathbb{E}(x)\mathbb{S}(x) - (x+\frac{1}{x})\mathbb{S}(x)\mathbb{O}(x),$$
$$\sum_{k>0} \text{rank } \mathcal{B}_{k,4}x^k \stackrel{?}{=} \mathbb{E}(x)\mathbb{O}(x)^3 - \frac{1}{x^2}\mathbb{E}(x)\mathbb{O}(x)\mathbb{S}(x) - (x+\frac{2}{x})\mathbb{S}(x)\mathbb{O}(x)^2 + (x+\frac{1}{x})\mathbb{S}(x)^2.$$

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