

Modular graph forms from equivariant iterated Eisenstein integrals

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ABSTRACT: The low-energy expansion of closed-string scattering amplitudes at genus one introduces infinite families of non-holomorphic modular forms called *modular graph forms*. Their differential and number-theoretic properties motivated Brown's alternative construction of non-holomorphic modular forms in the recent mathematics literature from so-called *equivariant iterated Eisenstein integrals*. In this work, we provide the first validations beyond depth one of Brown's conjecture that equivariant iterated Eisenstein integrals contain modular graph forms. Apart from a variety of examples at depth two and three, we spell out the systematics of the dictionary and make certain elements of Brown's construction fully explicit to all orders.

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1 Introduction

Scattering amplitudes in string theories have turned out to be rewarding laboratories to encounter deep mathematical structures in a physics context. Already at tree level, the multiple zeta values (MZVs) in the low-energy expansion of string amplitudes furnish elegant physics applications of motivic MZVs [1], the Drinfeld associator [2–5] and single-valued MZVs [1, 6–10]. At one loop, the common themes of string amplitudes, number theory, and algebraic geometry are centered around elliptic polylogarithms [11–14] and non-holomorphic modular forms. The latter arise from integrating over closed-string insertions on a torus [15–18] and were dubbed *modular graph forms* (MGFs) [19, 20]. We refer to [21] for an overview of MGFs as of fall 2020 and to [22–24] for recent discussions in a broader context.

The remarkable properties of MGFs attracted considerable attention among mathematicians, for instance, their intricate network of algebraic and differential relations [17, 20, 25–28] or the appearance of (conjecturally single-valued) MZVs in their Fourier expansion [19, 29–34]. In particular, the advent of MGFs inspired Brown’s construction of non-holomorphic modular forms from iterated integrals of holomorphic Eisenstein series and their complex conjugates [35–37]. More specifically, Brown’s infinite families of non-holomorphic modular forms arise as expansion coefficients of certain generating series dubbed *equivariant iterated Eisenstein integrals* (EIEIs) and are conjectured to contain MGFs.

Brown’s EIEIs are built from two implicitly defined ingredients [35, 37]: (i) a generating series b^{sv} of single-valued MZVs and (ii) a change of alphabet ϕ^{sv} for the bookkeeping variables of antiholomorphic iterated Eisenstein integrals akin to the construction of single-valued polylogarithms at genus zero in [38]. This close relation to the theory of single-valued polylogarithms is just one reason Brown’s non-holomorphic modular forms are of great interest across several communities. Other reasons include their potential application to solving arithmetic problems involving periods and their link to the study of universal mixed motives. Further recent evidence for their arithmetic significance was also provided by [39], where classical and important number-theoretic objects, such as period polynomials, were associated with the space of such non-holomorphic modular forms. Despite this interest, the explicit form of Brown’s EIEIs beyond depth one is essentially uncharted territory, apart from the simplest contributions of (i) to non-holomorphic Eisenstein series.

An explicit example of how MGFs at depth two relate to Brown’s non-holomorphic modular forms was given first in [36] and then further investigated in [40], where the depth-three case was also briefly discussed. However, the equations determining (i) and (ii) have not yet been solved to the orders that probe the generic properties of Brown’s non-holomorphic modular forms or their connection to MGFs at depth ≥ 2 .

An alternative way of reducing MGFs to iterated Eisenstein integrals and their complex conjugates was initiated by certain generating series of closed-string genus-one integrals which contain all convergent MGFs in their low-energy expansion [41]. The explicitly-known reality properties and first-order differential equations in τ of these closed-string integrals imply that MGFs can be uniquely expressed in terms of real-analytic iterated Eisenstein integrals β^{sv} [42]. These representations of MGFs expose both the entirety of their relations over rational combinations of MZVs and their expansion around the cusp.

The dictionary between MGFs and β^{sv} at depth two is known from [43, 44], and we will report on generalizations to depth three in future work [45].

In this work, we relate the organization of iterated Eisenstein integrals via β^{sv} to Brown’s construction of non-holomorphic modular forms and confirm his conjecture that EIEs contain MGFs in a variety of cases. Moreover, we present an all-order proposal for the explicit form of the aforementioned change of alphabet ϕ^{sv} in terms of commutator relations between certain derivations $\{\epsilon_{2k+2}, z_{2k+1}\}$ with $k \in \mathbb{N}$ which are well known in the mathematics literature. These derivations originated in pioneering work of Ihara [46], where deep connections to Grothendieck’s theory of motives (and particularly to Deligne’s motivic fundamental group of the projective line minus three points [47]) were found. The link between quadratic relations among these derivations and modular forms was first described by Ihara-Takao (see the summary in [48]), then studied in detail by Tsunogai [49], Goncharov [50], Gangl-Kaneko-Zagier [51], Schneps [52], Pollack [53], Baumard-Schneps [54], Hain-Matsumoto [55] and Brown [56, 57].

Our results close a notorious gap between the recent physics and mathematics literature and may pave the way for deducing properties of closed-string amplitudes from powerful theorems in algebraic geometry and number theory.

Outline. This work is organized as follows: we start by reviewing the basics of MGFs and their iterated-integral building blocks from the string-theory literature in section 2. Section 3 then introduces new results on these string-theory motivated building blocks with a focus on the construction of non-holomorphic modular forms. This description of MGFs is compared with Brown’s EIEs in section 4: we first make a connection with Brown’s generating series in terms of Tsunogai’s derivations [37] in subsections 4.1 and 4.2. The role of Brown’s equivariant double integrals including depth-one integrals of holomorphic cusp forms [35, 36] is then discussed in section 4.3.

2 Basics

We start by reviewing selected aspects of MGFs and setting up the notation to connect with Brown’s work in later sections.

2.1 Modular graph forms

The original definition of MGFs as integrals over marked points on a torus can be applied to any labeled directed graph [19, 20]. In lieu of the full definition, we restrict ourselves to simple instances that suffice to illustrate our construction. For the case of a dihedral graph, the definition of MGFs reduces to the following nested sums over discrete torus momenta p_1, \dots, p_R [20]

$$\mathcal{C}^+ \left[\begin{matrix} a_1 & \dots & a_R \\ b_1 & \dots & b_R \end{matrix} \right] (\tau) = \left(\prod_{j=1}^R \frac{(\text{Im } \tau)^{a_j}}{\pi^{b_j}} \right) \sum_{p_1, \dots, p_R \in \Lambda'} \frac{\delta(p_1 + \dots + p_R)}{p_1^{a_1} \bar{p}_1^{b_1} \dots p_R^{a_R} \bar{p}_R^{b_R}}. \tag{2.1}$$

MGFs depend non-holomorphically on the modular parameter $\tau \in \mathbb{C}$ of a torus with $\text{Im } \tau > 0$. The sums over lattice momenta

$$p_j \in \Lambda', \quad \Lambda' = (\mathbb{Z}\tau + \mathbb{Z}) \setminus \{0\} \tag{2.2}$$

converge absolutely if their exponents $a_j, b_j \in \mathbb{Z}$ obey $a_i + b_i + a_j + b_j \geq 3$ for all $1 \leq i < j \leq R$. The conventions for the normalization factor $(\text{Im } \tau)^{a_j} \pi^{-b_j}$ in (2.1) ensure that MGFs transform with purely antiholomorphic modular weight $(0, \sum_{j=1}^R (b_j - a_j))$ under the modular group $\text{SL}(2, \mathbb{Z})$,

$$\mathcal{C}^+ \begin{bmatrix} a_1 & \dots & a_R \\ b_1 & \dots & b_R \end{bmatrix} \left(\frac{a\tau + b}{c\bar{\tau} + d} \right) = \left(\prod_{j=1}^R (c\bar{\tau} + d)^{b_j - a_j} \right) \mathcal{C}^+ \begin{bmatrix} a_1 & \dots & a_R \\ b_1 & \dots & b_R \end{bmatrix} (\tau), \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z}). \quad (2.3)$$

Expressions similar to (2.1) for more general topologies are for instance discussed in [20, 58].

The simplest non-vanishing examples of MGFs are non-holomorphic Eisenstein series

$$E_k(\tau) = \mathcal{C}^+ \begin{bmatrix} k & 0 \\ k & 0 \end{bmatrix} (\tau) = \left(\frac{\text{Im } \tau}{\pi} \right)^k \sum_{p \in \Lambda'} \frac{1}{|p|^{2k}}, \quad k \geq 2 \quad (2.4)$$

and their $\tau, \bar{\tau}$ -derivatives. Infinitely many instances of (2.1) with $R \geq 3$ lattice momenta obey non-trivial relations such as [17, 25]

$$\begin{aligned} \mathcal{C}^+ \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} (\tau) &= E_3(\tau) + \zeta_3, \\ \mathcal{C}^+ \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} (\tau) &= 24\mathcal{C}^+ \begin{bmatrix} 2 & 1 & 1 \\ 2 & 1 & 1 \end{bmatrix} (\tau) - 18E_4(\tau) + 3E_2(\tau)^2, \end{aligned} \quad (2.5)$$

which are mysterious from the lattice-sum representations of MGFs but are exposed by the iterated-integral representations below. A datamine of relations can be found within the MATHEMATICA package [58]. Relations and expansions of MGFs around the cusp $\tau \rightarrow i\infty$ introduce (conjecturally single-valued [17, 29]) MZVs [26, 30–34]

$$\zeta_{n_1, n_2, \dots, n_r} = \sum_{0 < k_1 < k_2 < \dots < k_r} \frac{1}{k_1^{n_1} k_2^{n_2} \dots k_r^{n_r}}, \quad n_r \geq 2 \quad (2.6)$$

of weight $n_1 + n_2 + \dots + n_r$ and depth r .

2.2 Real-analytic iterated Eisenstein integrals

Non-holomorphic Eisenstein series (2.4) can be written as

$$E_k(\tau) = \frac{(2k-1)!}{(k-1)!^2} \left\{ -\beta^{\text{sv}} \left[\begin{matrix} k-1 \\ 2k \end{matrix}; \tau \right] + \frac{2\zeta_{2k-1}}{(2k-1)(4y)^{k-1}} \right\}, \quad (2.7)$$

involving the real-analytic depth-one integral [42, 43]

$$\begin{aligned} \beta^{\text{sv}} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right] &= \frac{1}{2\pi i} \left\{ \int_{\tau}^{i\infty} d\tau_1 \left(\frac{\tau - \tau_1}{4y} \right)^{k-2-j} (\bar{\tau} - \tau_1)^j G_k(\tau_1) \right. \\ &\quad \left. - \int_{\bar{\tau}}^{-i\infty} d\bar{\tau}_1 \left(\frac{\tau - \bar{\tau}_1}{4y} \right)^{k-2-j} (\bar{\tau} - \bar{\tau}_1)^j \overline{G_k(\tau_1)} \right\}, \end{aligned} \quad (2.8)$$

with $y = \pi \text{Im } \tau$, holomorphic Eisenstein series,

$$G_k(\tau) = (\text{Im } \tau)^{-k} \mathcal{C}^+ \begin{bmatrix} k & 0 \\ 0 & 0 \end{bmatrix} (\tau), \quad k \geq 4 \quad (2.9)$$

and tangential-basepoint regularization of the endpoint divergence at $\tau_1 \rightarrow i\infty$ [35]. Earlier discussions of iterated-integral representations of non-holomorphic Eisenstein series can for

instance be found in [17, 59]. We emphasize that the integrals in (2.8) and similar iterated integrals below are homotopy invariant: in spite of the appearance of τ and $\bar{\tau}$ in both lines, the integration variable τ_1 ($\bar{\tau}_1$) only appears holomorphically (antiholomorphically) along with $d\tau_1$ ($d\bar{\tau}_1$).

Generic MGFs (2.1) can be uniquely¹ represented via higher-depth generalizations of the real-analytic Eisenstein integral (2.8) which are constructed from kernels

$$\begin{aligned}\omega_+ \left[\begin{matrix} j \\ k \end{matrix}; \tau, \tau_1 \right] &= \frac{d\tau_1}{2\pi i} \left(\frac{\tau - \tau_1}{4y} \right)^{k-2-j} (\bar{\tau} - \tau_1)^j G_k(\tau_1), \\ \omega_- \left[\begin{matrix} j \\ k \end{matrix}; \tau, \tau_1 \right] &= -\frac{d\bar{\tau}_1}{2\pi i} \left(\frac{\tau - \bar{\tau}_1}{4y} \right)^{k-2-j} (\bar{\tau} - \bar{\tau}_1)^j \overline{G_k(\tau_1)},\end{aligned}\tag{2.10}$$

with $k \geq 4$ even and $0 \leq j \leq k-2$. In terms of these kernels, the depth-one expression (2.8) simply reads

$$\beta^{\text{sv}} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right] = \int_{\tau}^{i\infty} \omega_+ \left[\begin{matrix} j \\ k \end{matrix}; \tau, \tau_1 \right] + \int_{\bar{\tau}}^{-i\infty} \omega_- \left[\begin{matrix} j \\ k \end{matrix}; \tau, \tau_1 \right].\tag{2.11}$$

Starting from the depth-two instance [42, 43]

$$\begin{aligned}\beta^{\text{sv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right] &= \\ &\int_{\tau}^{i\infty} \omega_+ \left[\begin{matrix} j_2 \\ k_2 \end{matrix}; \tau, \tau_2 \right] \int_{\tau_2}^{i\infty} \omega_+ \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau, \tau_1 \right] + \int_{\tau}^{i\infty} \omega_+ \left[\begin{matrix} j_2 \\ k_2 \end{matrix}; \tau, \tau_2 \right] \int_{\bar{\tau}}^{-i\infty} \omega_- \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau, \tau_1 \right] \\ &+ \int_{\bar{\tau}}^{-i\infty} \omega_- \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau, \tau_1 \right] \int_{\bar{\tau}_1}^{-i\infty} \omega_- \left[\begin{matrix} j_2 \\ k_2 \end{matrix}; \tau, \tau_2 \right] + \sum_{p_1=0}^{k_1-2-j_1} \sum_{p_2=0}^{k_2-2-j_2} \frac{\binom{k_1-2-j_1}{p_1} \binom{k_2-2-j_2}{p_2}}{(4y)^{p_1+p_2}} \alpha \left[\begin{matrix} j_1+p_1 & j_2+p_2 \\ k_1 & k_2 \end{matrix}; \tau \right],\end{aligned}\tag{2.12}$$

the real-analytic β^{sv} involve antiholomorphic building blocks $\overline{\alpha[\dots; \tau]}$ featuring MZVs in each term which resemble the admixtures of MZVs to single-valued polylogarithms at genus zero in [38]. Just like the β^{sv} at arbitrary depth, the $\overline{\alpha[\dots; \tau]}$ are invariant under the modular T -transformation $\tau \rightarrow \tau+1$, see (3.21) below for an all-order formula at depth two. Note the reversal of the ordering of labels for the ω_- kernels in the definition (2.12).

The kernels (2.10) lead to specific linear combinations of Brown's iterated Eisenstein integrals over kernels $\tau_1^j G_k(\tau_1)$ with $k \geq 4$ and $0 \leq j \leq k-2$ [35]. Their accompanying polynomials in τ and $\bar{\tau}$ can be understood from their generating function

$$\begin{aligned}&\sum_{j=0}^{k-2} \omega_{\pm} \left[\begin{matrix} j \\ k \end{matrix}; \tau, \tau_1 \right] (X - \tau Y)^j (X - \bar{\tau} Y)^{k-j-2} \binom{k-2}{j} \frac{1}{(-4y)^j} \\ &= \begin{cases} \frac{d\tau_1}{(2\pi i)^{k-1}} (X - \tau_1 Y)^{k-2} G_k(\tau_1) : \omega_+, \\ -\frac{d\bar{\tau}_1}{(2\pi i)^{k-1}} (X - \bar{\tau}_1 Y)^{k-2} \overline{G_k(\tau_1)} : \omega_-, \end{cases},\end{aligned}\tag{2.13}$$

¹Uniqueness follows from the linear-independence results of [60] on holomorphic iterated Eisenstein integrals.

which translate into the kernels $(X - \tau_1 Y)^{k-2} G_k(\tau_1)$ of Brown's EIEIs [36]: once the commutative bookkeeping variables X, Y are taken to transform as a vector under $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z})$ according to $(X, Y) \rightarrow (aX + bY, cX + dY)$, both cases of (2.13) are modular invariant.

2.3 Higher-depth generalization

With a capital-letter notation P for words in the composite letters $\overset{j}{k}$ of the kernels (2.10), we can write the higher-depth generalization of (2.11) and (2.12) as

$$\beta^{\text{sv}}[P; \tau] = \sum_{P=XYZ} \overline{\kappa[X; \tau]} \beta_-[Y^t; \tau] \beta_+[Z; \tau], \tag{2.14}$$

where Y^t is obtained from Y by reversing the order of its composite letters (e.g. $\begin{pmatrix} j_1 & j_2 \\ k_2 & k_1 \end{pmatrix}^t = \begin{pmatrix} j_2 & j_1 \\ k_1 & k_2 \end{pmatrix}$), and the sum over deconcatenations of P into XYZ includes empty words X, Y, Z with $\overline{\kappa[\emptyset; \tau]} = \beta_-[\emptyset; \tau] = \beta_+[\emptyset; \tau] = 1$. We use a β_{\pm} -notation to separate the contributions from holomorphic and antiholomorphic Eisenstein series

$$\begin{aligned} \beta_+ \left[\begin{matrix} j_1 & j_2 & \dots & j_\ell \\ k_1 & k_2 & \dots & k_\ell \end{matrix}; \tau \right] &= \int_{\tau}^{i\infty} \omega_+ \left[\begin{matrix} j_\ell \\ k_\ell \end{matrix}; \tau, \tau_\ell \right] \dots \int_{\tau_3}^{i\infty} \omega_+ \left[\begin{matrix} j_2 \\ k_2 \end{matrix}; \tau, \tau_2 \right] \int_{\tau_2}^{i\infty} \omega_+ \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau, \tau_1 \right], \\ \beta_- \left[\begin{matrix} j_1 & j_2 & \dots & j_\ell \\ k_1 & k_2 & \dots & k_\ell \end{matrix}; \tau \right] &= \int_{\bar{\tau}}^{-i\infty} \omega_- \left[\begin{matrix} j_\ell \\ k_\ell \end{matrix}; \tau, \tau_\ell \right] \dots \int_{\bar{\tau}_3}^{-i\infty} \omega_- \left[\begin{matrix} j_2 \\ k_2 \end{matrix}; \tau, \tau_2 \right] \int_{\bar{\tau}_2}^{-i\infty} \omega_- \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau, \tau_1 \right]. \end{aligned} \tag{2.15}$$

Moreover, the composition of antiholomorphic $\overline{\alpha[\dots; \tau]}$ in the last line of (2.12) generalizes to multiple sums over p_i ,

$$\overline{\kappa \left[\begin{matrix} \dots & j_i & \dots \\ \dots & k_i & \dots \end{matrix}; \tau \right]} = \sum_{p_i=0}^{k_i-2-j_i} \frac{\binom{k_i-2-j_i}{p_i}}{(4y)^{p_i}} \overline{\alpha \left[\begin{matrix} \dots & j_i+p_i & \dots \\ \dots & k_i & \dots \end{matrix}; \tau \right]}, \tag{2.16}$$

where one can infer the vanishing of their depth-one instances $\overline{\kappa \left[\begin{matrix} j \\ k \end{matrix}; \tau \right]} = \overline{\alpha \left[\begin{matrix} j \\ k \end{matrix}; \tau \right]} = 0$ from (2.8). Antiholomorphicity of the $\overline{\alpha[\dots; \tau]}$ and the composition rule (2.14) imply a simple form of the holomorphic differential equations [42]

$$\begin{aligned} 2\pi i(\tau - \bar{\tau})^2 \partial_\tau \beta^{\text{sv}} \left[\begin{matrix} j_1 & \dots & j_\ell \\ k_1 & \dots & k_\ell \end{matrix}; \tau \right] &= \sum_{i=1}^{\ell} (k_i - j_i - 2) \beta^{\text{sv}} \left[\begin{matrix} j_1 & \dots & j_i+1 & \dots & j_\ell \\ k_1 & \dots & k_i & \dots & k_\ell \end{matrix}; \tau \right] \\ &\quad - \delta_{j_\ell, k_\ell - 2} (\tau - \bar{\tau})^{k_\ell} G_{k_\ell}(\tau) \beta^{\text{sv}} \left[\begin{matrix} j_1 & \dots & j_{\ell-1} \\ k_1 & \dots & k_{\ell-1} \end{matrix}; \tau \right], \end{aligned} \tag{2.17}$$

while $\partial_{\bar{\tau}}$ -derivatives are in general more complicated and sensitive to the expressions for $\overline{\alpha[\dots; \tau]}$.

Note that all the $\overline{\kappa[X; \tau]}$ and the combinations $\sum_{Q=YZ} \beta_-[Y^t; \tau] \beta_+[Z; \tau]$ in (2.14) at fixed Q are separately invariant under $T : \tau \rightarrow \tau + 1$. Modular S -transformations $\tau \rightarrow -\frac{1}{\tau}$ in turn mix β^{sv} of different depths [42, 44] with rational functions of $\tau, \bar{\tau}$, MZVs and more general multiple modular values [35, 61] in their coefficients. In other words, individual β^{sv} do not have good modular properties, unlike MGFs, which are specific linear combinations of β^{sv} of different depths with y -dependent coefficients. One of the main aims of this paper is to give a more direct characterization of these linear combinations (see section 3) and to relate them to Brown's construction in section 4.

2.4 Generating series of modular graph forms

The entirety of convergent MGFs which do not simplify under holomorphic subgraph reduction [20, 28] are embedded into generating series of closed-string integrals over $n \geq 2$ marked points on a torus [41]. Their KZB-type differential equations in τ have been solved through a generating series in β^{sv} [42]

$$Y_{\vec{\eta}}^{\tau} = \sum_P R_{\vec{\eta}}(\epsilon[P]) \beta^{\text{sv}}[P; \tau] \exp\left(-\frac{R_{\vec{\eta}}(\epsilon_0)}{4y}\right) \widehat{Y}_{\vec{\eta}}^{i\infty}, \quad (2.18)$$

where we recall $y = \pi \text{Im } \tau$, and the sum over P comprises all words $P = \frac{j_1 \dots j_\ell}{k_1 \dots k_\ell}$ of length $\ell \geq 0$ with $k_i \geq 4$ even and $0 \leq j_i \leq k_i - 2$. The coefficients

$$\epsilon \left[\begin{matrix} j_1 & j_2 & \dots & j_\ell \\ k_1 & k_2 & \dots & k_\ell \end{matrix} \right] = \left(\prod_{i=1}^{\ell} \frac{(-1)^{j_i} (k_i - 1)}{(k_i - j_i - 2)!} \right) \epsilon_{k_\ell}^{(k_\ell - 2 - j_\ell)} \dots \epsilon_{k_2}^{(k_2 - 2 - j_2)} \epsilon_{k_1}^{(k_1 - 2 - j_1)} \quad (2.19)$$

with the shorthand

$$\epsilon_k^{(j)} = \text{ad}_{\epsilon_0}^j(\epsilon_k) \quad (2.20)$$

and the exponential in (2.18) involve certain $(n-1)! \times (n-1)!$ matrix valued operators $R_{\vec{\eta}}(\epsilon_{k \in 2\mathbb{N}_0})$ which are conjectured [41, 42] to furnish matrix representations $R_{\vec{\eta}}(\cdot)$ of Tsunogai's derivation algebra $\{\epsilon_{k \in 2\mathbb{N}_0}\}$ [49] with $R_{\vec{\eta}}(\epsilon_2) = 0$. The notation $R_{\vec{\eta}}(\epsilon[P])$ in (2.18) instructs us to replace all the ϵ_k in (2.19) by $R_{\vec{\eta}}(\epsilon_k)$. The conjecture is supported by a huge number of checks that the relations of the derivation algebra [49, 53, 62] such as

$$\begin{aligned} 0 &= \epsilon_k^{(k-1)}, & k \geq 4 \text{ even}, \\ 0 &= [\epsilon_4, \epsilon_{10}] - 3[\epsilon_6, \epsilon_8], \\ 0 &= -462[\epsilon_4, [\epsilon_4, \epsilon_8]] - 1725[\epsilon_6, [\epsilon_6, \epsilon_4]] - 280[\epsilon_8, \epsilon_8^{(1)}] \\ &\quad + 125[\epsilon_6, \epsilon_{10}^{(1)}] + 250[\epsilon_{10}, \epsilon_6^{(1)}] - 80[\epsilon_{12}, \epsilon_4^{(1)}] - 16[\epsilon_4, \epsilon_{12}^{(1)}] \end{aligned} \quad (2.21)$$

are preserved in passing to the matrix-valued operators $\epsilon_k \rightarrow R_{\vec{\eta}}(\epsilon_k)$.

Finally, the quantity $\widehat{Y}_{\vec{\eta}}^{i\infty}$ in (2.18) accounts for the $\tau \rightarrow i\infty$ degenerations of the genus-one integrals [41, 42]. Its matrix entries are τ -independent Laurent series in the bookkeeping variables s_{ij}, η_j of the reference that the operators $R_{\vec{\eta}}(\epsilon_k)$ act on, with (conjecturally single-valued) MZVs in their coefficients (the explicit form at $n = 2$ can be generated from (4.2) of [42]).

2.5 Examples

The contributions of $\exp\left(-\frac{R_{\vec{\eta}}(\epsilon_0)}{4y}\right) \widehat{Y}_{\vec{\eta}}^{i\infty}$ to the generating series (2.18) ensure that β^{sv} of different depths are combined into modular forms. At depth one, the formula is [42]

$$C^+ \left[\begin{matrix} a & 0 \\ b & 0 \end{matrix} \right] (\tau) = -\frac{(2i)^{b-a} (a+b-1)!}{(a-1)! (b-1)!} \left(\beta^{\text{sv}} \left[\begin{matrix} a-1 \\ a+b \end{matrix}; \tau \right] - \frac{2\zeta_{a+b-1}}{(a+b-1)(4y)^{b-1}} \right), \quad (2.22)$$

where $a, b \geq 1$, and $a+b \geq 4$ is an even integer.

Higher-depth instances of β^{sv} in (2.12) and (2.14) occur in MGFs with three and more columns, such as [42]

$$\begin{aligned} \mathcal{C}^+[\begin{smallmatrix} 2 & 1 & 1 \\ 2 & 1 & 1 \end{smallmatrix}](\tau) &= -126\beta^{\text{sv}}[\begin{smallmatrix} 3 \\ 8 \end{smallmatrix}; \tau] - 18\beta^{\text{sv}}[\begin{smallmatrix} 2 & 0 \\ 4 & 4 \end{smallmatrix}; \tau] + 12\zeta_3\beta^{\text{sv}}[\begin{smallmatrix} 0 \\ 4 \end{smallmatrix}; \tau] + \frac{5\zeta_5}{12y} - \frac{\zeta_3^2}{4y^2} + \frac{9\zeta_7}{16y^3}, \\ \mathcal{C}^+[\begin{smallmatrix} 3 & 2 & 1 \\ 1 & 2 & 1 \end{smallmatrix}](\tau) &= \frac{279}{2}\beta^{\text{sv}}[\begin{smallmatrix} 5 \\ 10 \end{smallmatrix}; \tau] + 30\beta^{\text{sv}}[\begin{smallmatrix} 3 & 1 \\ 6 & 4 \end{smallmatrix}; \tau] + \frac{15}{2}\beta^{\text{sv}}[\begin{smallmatrix} 4 & 0 \\ 6 & 4 \end{smallmatrix}; \tau] \\ &\quad - 3\zeta_5\beta^{\text{sv}}[\begin{smallmatrix} 0 \\ 4 \end{smallmatrix}; \tau] - \frac{3\zeta_5}{y}\beta^{\text{sv}}[\begin{smallmatrix} 1 \\ 4 \end{smallmatrix}; \tau] - \frac{7\zeta_7}{48y} + \frac{5\zeta_3\zeta_5}{16y^2} - \frac{31\zeta_9}{64y^3} \end{aligned} \quad (2.23)$$

as well as [42]

$$\begin{aligned} 2i\text{Im}\mathcal{C}^+[\begin{smallmatrix} 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 3 \end{smallmatrix}](\tau) &= 60\beta^{\text{sv}}[\begin{smallmatrix} 0 & 3 \\ 4 & 6 \end{smallmatrix}; \tau] - 270\beta^{\text{sv}}[\begin{smallmatrix} 1 & 2 \\ 4 & 6 \end{smallmatrix}; \tau] - 60\beta^{\text{sv}}[\begin{smallmatrix} 1 & 2 \\ 6 & 4 \end{smallmatrix}; \tau] + 390\beta^{\text{sv}}[\begin{smallmatrix} 2 & 1 \\ 4 & 6 \end{smallmatrix}; \tau] \\ &\quad + 270\beta^{\text{sv}}[\begin{smallmatrix} 2 & 1 \\ 6 & 4 \end{smallmatrix}; \tau] - 390\beta^{\text{sv}}[\begin{smallmatrix} 3 & 0 \\ 6 & 4 \end{smallmatrix}; \tau] - 3\zeta_3\beta^{\text{sv}}[\begin{smallmatrix} 1 \\ 4 \end{smallmatrix}; \tau] + \frac{39\zeta_5}{y}\beta^{\text{sv}}[\begin{smallmatrix} 0 \\ 4 \end{smallmatrix}; \tau] \\ &\quad - \frac{27\zeta_5}{4y^2}\beta^{\text{sv}}[\begin{smallmatrix} 1 \\ 4 \end{smallmatrix}; \tau] + \frac{3\zeta_5}{8y^3}\beta^{\text{sv}}[\begin{smallmatrix} 2 \\ 4 \end{smallmatrix}; \tau] - 260\zeta_3\beta^{\text{sv}}[\begin{smallmatrix} 1 \\ 6 \end{smallmatrix}; \tau] + \frac{45\zeta_3}{y}\beta^{\text{sv}}[\begin{smallmatrix} 2 \\ 6 \end{smallmatrix}; \tau] \\ &\quad - \frac{5\zeta_3}{2y^2}\beta^{\text{sv}}[\begin{smallmatrix} 3 \\ 6 \end{smallmatrix}; \tau] - \frac{13\zeta_5}{120}. \end{aligned} \quad (2.24)$$

As a common theme of (2.22) to (2.24), $\beta^{\text{sv}}[\begin{smallmatrix} j_1 & \dots & j_\ell \\ k_1 & \dots & k_\ell \end{smallmatrix}; \tau]$ are completed to modular forms of weight $(0, \sum_{i=1}^\ell (k_i - 2 - 2j_i))$ by adding lower-depth terms with $\mathbb{Q}[y^{-1}]$ -linear combinations of MZVs in their coefficients. Note that only non-positive powers of y can arise from the expansion of the exponential in (2.18).

The antiholomorphic $\overline{\alpha[\dots; \tau]}$ in (2.12) and at higher depth are determined by the reality properties

$$\overline{\mathcal{C}^+[\begin{smallmatrix} a_1 & \dots & a_R \\ b_1 & \dots & b_R \end{smallmatrix}](\tau)} = \left(\prod_{r=1}^R y^{a_r - b_r} \right) \mathcal{C}^+[\begin{smallmatrix} b_1 & \dots & b_R \\ a_1 & \dots & a_R \end{smallmatrix}](\tau), \quad (2.25)$$

once a β^{sv} representation of all basis MGFs at given weight $\sum_{r=1}^R (a_r + b_r)$ is available. Examples and general formulae at depth two will be given in the next section (also see appendix A).

3 Modular forms from β^{sv}

In this section, we describe the structure of modular forms constructed from β^{sv} in preparation for the matching with Brown's EIEIs. These modular versions will be denoted by β^{eqv} by slight abuse of notation since they are not equivariant but simply standard non-holomorphic modular forms. Since the β^{sv} and their y -dependent coefficients are invariant under T -transformations, we only need to ensure that the S -modular transformation law is correct.

The answer at depth one is straightforward to obtain since the modular S -transformation of (2.8) involves a depth-zero term which cancels from the combination

$$\beta^{\text{eqv}}\left[\begin{smallmatrix} j \\ k \end{smallmatrix}; \tau\right] = \beta^{\text{sv}}\left[\begin{smallmatrix} j \\ k \end{smallmatrix}; \tau\right] - \frac{2\zeta_{k-1}}{(k-1)(4y)^{k-j-2}}. \quad (3.1)$$

This illustrates the fact that the β^{sv} have to be completed by lower-depth terms with non-positive powers of y and (single-valued) MZVs.

3.1 Construction and properties of β^{eqv}

Modular versions of $\beta^{\text{sv}}[P; \tau]$ as seen in (2.22) to (2.24) can be parameterized by constants $c^{\text{sv}}[P]$ associated with the same type of words P in composite letters $\overset{j}{k}$ with $k \geq 4$ even and $0 \leq j \leq k-2$,

$$\begin{aligned} \beta^{\text{eqv}}\left[\overset{j}{k}; \tau\right] &= \beta^{\text{sv}}\left[\overset{j}{k}; \tau\right] + \sum_{p=0}^{k-j-2} \frac{\binom{k-j-2}{p}}{(4y)^p} c^{\text{sv}}\left[\overset{j+p}{k}\right], \\ \beta^{\text{eqv}}\left[\overset{j_1}{k_1} \overset{j_2}{k_2}; \tau\right] &= \beta^{\text{sv}}\left[\overset{j_1}{k_1} \overset{j_2}{k_2}; \tau\right] + \sum_{p_1=0}^{k_1-j_1-2} \frac{\binom{k_1-j_1-2}{p_1}}{(4y)^{p_1}} c^{\text{sv}}\left[\overset{j_1+p_1}{k_1}\right] \beta^{\text{sv}}\left[\overset{j_2}{k_2}; \tau\right] \\ &+ \sum_{p_1=0}^{k_1-j_1-2} \sum_{p_2=0}^{k_2-j_2-2} \frac{\binom{k_1-j_1-2}{p_1} \binom{k_2-j_2-2}{p_2}}{(4y)^{p_1+p_2}} c^{\text{sv}}\left[\overset{j_1+p_1}{k_1} \overset{j_2+p_2}{k_2}\right] + \beta_{\Delta}^{\text{sv}}\left[\overset{j_1}{k_1} \overset{j_2}{k_2}; \tau\right], \end{aligned} \quad (3.2)$$

and more generally

$$\beta^{\text{eqv}}[P; \tau] = \beta_{\Delta}^{\text{sv}}[P; \tau] + \sum_{P=XY} d^{\text{sv}}[X; \tau] \beta^{\text{sv}}[Y; \tau], \quad (3.3)$$

where the constants c^{sv} have been reassembled into polynomials in y^{-1} ,

$$d^{\text{sv}}\left[\dots \overset{j_i}{k_i} \dots; \tau\right] = \sum_{p_i=0}^{k_i-2-j_i} \frac{\binom{k_i-2-j_i}{p_i}}{(4y)^{p_i}} c^{\text{sv}}\left[\dots \overset{j_i+p_i}{k_i} \dots\right], \quad (3.4)$$

and we again have one summation of this type per column. The $\beta_{\Delta}^{\text{sv}}$ appearing in (3.2) are iterated integrals with at least one holomorphic cusp form $\Delta_{2s}(\tau)$ among its kernels. They do not contribute to MGFs [20, 28, 41], vanish at depth one, i.e. $\beta_{\Delta}^{\text{sv}}\left[\overset{j}{k}; \tau\right] = 0$, and will be discussed in section 3.4. Up to these cusp-form contributions, the differential equations

$$\begin{aligned} 2\pi i(\tau - \bar{\tau})^2 \partial_{\tau} \beta^{\text{eqv}}\left[\overset{j_1}{k_1} \dots \overset{j_{\ell}}{k_{\ell}}; \tau\right] &= \sum_{i=1}^{\ell} (k_i - j_i - 2) \beta^{\text{eqv}}\left[\overset{j_1}{k_1} \dots \overset{j_i+1}{k_i} \dots \overset{j_{\ell}}{k_{\ell}}; \tau\right] \\ &- \delta_{j_{\ell}, k_{\ell}-2} (\tau - \bar{\tau})^{k_{\ell}} G_{k_{\ell}}(\tau) \beta^{\text{eqv}}\left[\overset{j_1}{k_1} \dots \overset{j_{\ell-1}}{k_{\ell-1}}; \tau\right] \bmod \beta_{\Delta}^{\text{sv}} \end{aligned} \quad (3.5)$$

take the same form as those of the β^{sv} in (2.17) [42].

A few comments on the equations above are in order. Firstly, we stress that the combination of $(4y)^{-1}$ with constants $c^{\text{sv}}[\dots]$ in (3.3) or $\overline{\alpha}[\dots; \tau]$ in (2.16) both preserve the form of (3.5). Secondly, we notice that the construction (3.3) of $\beta^{\text{eqv}}[P; \tau]$ is expressed in terms of $d^{\text{sv}}[X; \tau] \beta^{\text{sv}}[Y; \tau]$ with deconcatenations $P = XY$ of the word P , such that $\beta^{\text{sv}}[Y; \tau]$ is precisely labelled by the second subword Y . This fact ensures that only the right-most letter $\overset{j_{\ell}}{k_{\ell}}$ of P causes the appearance of holomorphic Eisenstein integration kernels in (3.5).

Once the constants c^{sv} and the T -invariant cusp-form contributions $\beta_{\Delta}^{\text{sv}}$ are tailored to the multiple modular values in the S -transformations of (2.15), the β^{eqv} in (3.3) transform as non-holomorphic modular forms

$$\beta^{\text{eqv}}\left[\overset{j_1}{k_1} \dots \overset{j_{\ell}}{k_{\ell}}; \frac{a\tau+b}{c\tau+d}\right] = \left(\prod_{i=1}^{\ell} (c\bar{\tau}+d)^{k_i-2-2j_i}\right) \beta^{\text{eqv}}\left[\overset{j_1}{k_1} \dots \overset{j_{\ell}}{k_{\ell}}; \tau\right], \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z}). \quad (3.6)$$

The constants $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & \dots & j_\ell \\ k_1 & \dots & k_\ell \end{smallmatrix} \right]$ are (conjecturally single-valued) MZVs (2.6) of weight $\sum_{i=1}^{\ell} (j_i+1)$. The earlier expression (3.1) for $\beta^{\text{eqv}} \left[\begin{smallmatrix} j \\ k \end{smallmatrix} ; \tau \right]$ at depth one implies the closed formulae

$$c^{\text{sv}} \left[\begin{smallmatrix} j \\ k \end{smallmatrix} \right] = -\frac{2\zeta_{k-1}}{k-1} \delta_{j,k-2}, \quad d^{\text{sv}} \left[\begin{smallmatrix} j \\ k \end{smallmatrix} ; \tau \right] = -\frac{2\zeta_{k-1}}{(k-1)(4y)^{k-2-j}}. \quad (3.7)$$

At depth two, all the $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$ with $k_1+k_2 \leq 28$ and $0 \leq j_i \leq k_i-2$ are fixed by the β^{sv} -representations of certain modular invariants $F_{m,k}^{\pm(s)}$ and their $\tau, \bar{\tau}$ -derivatives at $m+k \leq 14$ in the ancillary files of [43, 44]. Double integrals of $G_4(\tau_1)G_4(\tau_2)$ give rise to constants

$$\begin{aligned} c^{\text{sv}} \left[\begin{smallmatrix} 0 & 0 \\ 4 & 4 \end{smallmatrix} \right] &= 0, & c^{\text{sv}} \left[\begin{smallmatrix} 0 & 1 \\ 4 & 4 \end{smallmatrix} \right] &= -\frac{\zeta_3}{2160}, & c^{\text{sv}} \left[\begin{smallmatrix} 0 & 2 \\ 4 & 4 \end{smallmatrix} \right] &= 0, \\ c^{\text{sv}} \left[\begin{smallmatrix} 1 & 0 \\ 4 & 4 \end{smallmatrix} \right] &= \frac{\zeta_3}{2160}, & c^{\text{sv}} \left[\begin{smallmatrix} 1 & 1 \\ 4 & 4 \end{smallmatrix} \right] &= 0, & c^{\text{sv}} \left[\begin{smallmatrix} 1 & 2 \\ 4 & 4 \end{smallmatrix} \right] &= \frac{5\zeta_5}{108}, \\ c^{\text{sv}} \left[\begin{smallmatrix} 2 & 0 \\ 4 & 4 \end{smallmatrix} \right] &= 0, & c^{\text{sv}} \left[\begin{smallmatrix} 2 & 1 \\ 4 & 4 \end{smallmatrix} \right] &= -\frac{5\zeta_5}{108}, & c^{\text{sv}} \left[\begin{smallmatrix} 2 & 2 \\ 4 & 4 \end{smallmatrix} \right] &= \frac{2}{9}\zeta_3^2, \end{aligned} \quad (3.8)$$

and the non-vanishing instances of $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ 4 & 6 \end{smallmatrix} \right]$ are

$$\begin{aligned} c^{\text{sv}} \left[\begin{smallmatrix} 0 & 1 \\ 4 & 6 \end{smallmatrix} \right] &= \frac{\zeta_3}{907200}, & c^{\text{sv}} \left[\begin{smallmatrix} 1 & 0 \\ 4 & 6 \end{smallmatrix} \right] &= -\frac{\zeta_3}{226800}, \\ c^{\text{sv}} \left[\begin{smallmatrix} 0 & 3 \\ 4 & 6 \end{smallmatrix} \right] &= -\frac{\zeta_5}{7200}, & c^{\text{sv}} \left[\begin{smallmatrix} 1 & 2 \\ 4 & 6 \end{smallmatrix} \right] &= \frac{\zeta_5}{21600}, & c^{\text{sv}} \left[\begin{smallmatrix} 2 & 1 \\ 4 & 6 \end{smallmatrix} \right] &= -\frac{\zeta_5}{21600}, \\ c^{\text{sv}} \left[\begin{smallmatrix} 0 & 4 \\ 4 & 6 \end{smallmatrix} \right] &= -\frac{\zeta_3^2}{315}, & c^{\text{sv}} \left[\begin{smallmatrix} 1 & 3 \\ 4 & 6 \end{smallmatrix} \right] &= \frac{\zeta_3^2}{1260}, & c^{\text{sv}} \left[\begin{smallmatrix} 2 & 2 \\ 4 & 6 \end{smallmatrix} \right] &= -\frac{\zeta_3^2}{1890}, \\ c^{\text{sv}} \left[\begin{smallmatrix} 1 & 4 \\ 4 & 6 \end{smallmatrix} \right] &= \frac{7\zeta_7}{360}, & c^{\text{sv}} \left[\begin{smallmatrix} 2 & 3 \\ 4 & 6 \end{smallmatrix} \right] &= -\frac{7\zeta_7}{720}, & c^{\text{sv}} \left[\begin{smallmatrix} 2 & 4 \\ 4 & 6 \end{smallmatrix} \right] &= \frac{2\zeta_3\zeta_5}{15}. \end{aligned} \quad (3.9)$$

More general examples $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$ are composed of odd Riemann zeta values and bilinears thereof. A variety of $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix} \right]$ to be extracted from depth-three analogues of $F_{m,k}^{\pm(s)}$ in future work [45] involve indecomposable single-valued MZVs of depth three, such as

$$\begin{aligned} c^{\text{sv}} \left[\begin{smallmatrix} 2 & 2 & 4 \\ 4 & 4 & 6 \end{smallmatrix} \right] &= -\frac{1}{450}\zeta_{3,5,3}^{\text{sv}} - \frac{2}{45}\zeta_3^2\zeta_5 - \frac{221}{21600}\zeta_{11}, \\ c^{\text{sv}} \left[\begin{smallmatrix} 2 & 4 & 4 \\ 4 & 6 & 6 \end{smallmatrix} \right] &= \frac{1}{3750}\zeta_{5,3,5}^{\text{sv}} + \frac{2}{375}\zeta_3\zeta_5^2 + \frac{1804427}{124380000}\zeta_{13}, \\ c^{\text{sv}} \left[\begin{smallmatrix} 2 & 2 & 6 \\ 4 & 4 & 8 \end{smallmatrix} \right] &= -\frac{1}{1764}\zeta_{3,7,3}^{\text{sv}} + \frac{1}{1470}\zeta_{5,3,5}^{\text{sv}} - \frac{2}{63}\zeta_3^2\zeta_7 - \frac{137359}{24378480}\zeta_{13}, \end{aligned} \quad (3.10)$$

where [63, 64]

$$\begin{aligned} \zeta_{3,5,3}^{\text{sv}} &= 2\zeta_{3,5,3} - 2\zeta_3\zeta_{3,5} - 10\zeta_3^2\zeta_5, \\ \zeta_{5,3,5}^{\text{sv}} &= 2\zeta_{5,3,5} - 22\zeta_{3,5}\zeta_5 - 120\zeta_5^2\zeta_3 - 10\zeta_5\zeta_8, \\ \zeta_{3,7,3}^{\text{sv}} &= 2\zeta_{3,7,3} - 2\zeta_{3,7}\zeta_3 - 28\zeta_3^2\zeta_7 - 24\zeta_{3,5}\zeta_5 - 144\zeta_5^2\zeta_3 - 12\zeta_5\zeta_8. \end{aligned} \quad (3.11)$$

A list of all $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$ at $k_1+k_2 \leq 28$ and $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix} \right]$ with $k_1+k_2+k_3 \leq 16$ can be found in the supplementary material attached to this paper, and their instances with $j_i = k_i-2$ are revisited in the light of the f -alphabet in section 4.1.4.

As will be detailed in sections 4.1.2 and 4.3.3, some of the $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix} \right]$ at $j_1+j_2+j_3 = \frac{1}{2}(k_1+k_2+k_3) - 3$ and $k_1+k_2+k_3 \leq 16$ admit redefinitions that one may be able to fix from depth-four computations. We will track the one-parameter freedom $\sim c_{446}\zeta_7$ of $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 4 & 6 \end{smallmatrix} \right]$

and $\sim c_{466}\zeta_3\zeta_5$ of $c^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 6 & 6 \end{smallmatrix}\right]$ (with $c_{446}, c_{466} \in \mathbb{Q}$) in the supplementary material that amounts to shifting certain combinations of modular invariant $\beta^{\text{eqv}}\left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 4 & 6 \end{smallmatrix}\right]$ and $\beta^{\text{eqv}}\left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 6 & 6 \end{smallmatrix}\right]$ in an $\text{SL}(2, \mathbb{R})$ -singlet by constants.

All of $\beta^{\text{sv}}, \beta^{\text{eqv}}$ and c^{sv} are expected to obey shuffle relations inherited from iterated integrals such as

$$c^{\text{sv}}\left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] c^{\text{sv}}\left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}\right] = c^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right] + c^{\text{sv}}\left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right] \tag{3.12}$$

and more generally

$$\begin{aligned} \beta^{\text{sv}}[X; \tau] \beta^{\text{sv}}[Y; \tau] &= \sum_{P \in X \sqcup Y} \beta^{\text{sv}}[P; \tau], \\ \beta^{\text{eqv}}[X; \tau] \beta^{\text{eqv}}[Y; \tau] &= \sum_{P \in X \sqcup Y} \beta^{\text{eqv}}[P; \tau], \\ c^{\text{sv}}[X] c^{\text{sv}}[Y] &= \sum_{P \in X \sqcup Y} c^{\text{sv}}[P], \end{aligned} \tag{3.13}$$

with $X \sqcup Y$ denoting the shuffle product of the words X and Y . These shuffle relations are consequences of our central claim in (4.2) below that the modular forms β^{eqv} can be alternatively generated from Brown’s EIEIs.

3.2 Modular graph forms and beyond in terms of β^{eqv}

As will be illustrated from the examples in this section, the non-holomorphic modular forms β^{eqv} compactly encode iterated-integral representations of MGFs and more general modular forms. More specifically, each MGF can be written as a $\mathbb{Q}[\text{MZV}]$ -linear (conjecturally $\mathbb{Q}[\text{single-valued MZV}]$ -linear) combination of β^{eqv} , though there are β^{eqv} with contributions from holomorphic cusp forms which cannot be realized via MGFs.

The two-column cases (2.22) take the form

$$\mathcal{C}^+\left[\begin{smallmatrix} a & 0 \\ b & 0 \end{smallmatrix}\right] = -\frac{(2i)^{b-a}(a+b-1)!}{(a-1)!(b-1)!} \beta^{\text{eqv}}\left[\begin{smallmatrix} a-1 \\ a+b \end{smallmatrix}\right] \tag{3.14}$$

upon inserting the β^{eqv} at depth one into (3.1). The depth-two examples in (2.23) and (2.24) condense to

$$\begin{aligned} \mathcal{C}^+\left[\begin{smallmatrix} 2 & 1 & 1 \\ 2 & 1 & 1 \end{smallmatrix}\right] &= -126\beta^{\text{eqv}}\left[\begin{smallmatrix} 3 \\ 8 \end{smallmatrix}\right] - 18\beta^{\text{eqv}}\left[\begin{smallmatrix} 2 & 0 \\ 4 & 4 \end{smallmatrix}\right], \\ \mathcal{C}^+\left[\begin{smallmatrix} 3 & 2 & 1 \\ 1 & 2 & 1 \end{smallmatrix}\right] &= \frac{279}{2}\beta^{\text{eqv}}\left[\begin{smallmatrix} 5 \\ 10 \end{smallmatrix}\right] + 30\beta^{\text{eqv}}\left[\begin{smallmatrix} 3 & 1 \\ 6 & 4 \end{smallmatrix}\right] + \frac{15}{2}\beta^{\text{eqv}}\left[\begin{smallmatrix} 4 & 0 \\ 6 & 4 \end{smallmatrix}\right], \\ 2i \text{Im } \mathcal{C}^+\left[\begin{smallmatrix} 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 3 \end{smallmatrix}\right] &= 60(\beta^{\text{eqv}}\left[\begin{smallmatrix} 0 & 3 \\ 4 & 6 \end{smallmatrix}\right] - \beta^{\text{eqv}}\left[\begin{smallmatrix} 1 & 2 \\ 6 & 4 \end{smallmatrix}\right]) - 270(\beta^{\text{eqv}}\left[\begin{smallmatrix} 1 & 2 \\ 4 & 6 \end{smallmatrix}\right] - \beta^{\text{eqv}}\left[\begin{smallmatrix} 2 & 1 \\ 6 & 4 \end{smallmatrix}\right]) \\ &\quad + 390(\beta^{\text{eqv}}\left[\begin{smallmatrix} 2 & 1 \\ 4 & 6 \end{smallmatrix}\right] - \beta^{\text{eqv}}\left[\begin{smallmatrix} 3 & 0 \\ 6 & 4 \end{smallmatrix}\right]) - 3\zeta_3\beta^{\text{eqv}}\left[\begin{smallmatrix} 1 \\ 4 \end{smallmatrix}\right], \end{aligned} \tag{3.15}$$

by virtue of the $c^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ 4 & 6 \end{smallmatrix}\right]$ in (3.9) and the $c^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ 6 & 4 \end{smallmatrix}\right]$ following from the shuffle relations (3.12).

As a convenient organization of modular graph double integrals, certain modular invariant solutions $F_{m,k}^{\pm(s)}$ to inhomogeneous Laplace equations have been studied in [43, 44], with $2 \leq m \leq k$ referring to the E_m, E_k in the inhomogeneous terms. The real ones $F_{m,k}^{+(s)}$ are characterized by Laplace eigenvalues $s(s-1)$ with $s \in \{k-m+2, k-m+4, \dots, k+m-4, k+m-2\}$

and contain the three-column MGFs $\mathcal{C}^+ \begin{bmatrix} a & b & c \\ a & b & c \end{bmatrix}$ whose Laplace equations can be found in [17]. The imaginary ones $F_{m,k}^{-(s)}$ with $s \in \{k-m+1, k-m+3, \dots, k+m-3, k+m-1\}$ contain cuspidal MGFs with three or more columns such as $\text{Im } \mathcal{C}^+ \begin{bmatrix} 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 3 \end{bmatrix}$ in (3.15).

The collection of $\beta^{\text{eqv}} \begin{bmatrix} j_1 & j_2 \\ 2m & 2k \end{bmatrix}$ and $\beta^{\text{eqv}} \begin{bmatrix} j_2 & j_1 \\ 2k & 2m \end{bmatrix}$ with $0 \leq j_1 \leq 2m-2$ and $0 \leq j_2 \leq 2k-2$ can be expressed in terms of $F_{m,k}^{\pm(s)}$, bilinears in E_m, E_k , products $\zeta_{2m-1} E_s$ as well as respective modular derivatives $\nabla_\tau = 2i(\text{Im } \tau)^2 \partial_\tau$ and $\bar{\nabla}_\tau = -2i(\text{Im } \tau)^2 \partial_{\bar{\tau}}$. Conversely, we have compact identities

$$\begin{aligned} F_{2,2}^{+(2)} &= 18\beta^{\text{eqv}} \begin{bmatrix} 2 & 0 \\ 4 & 4 \end{bmatrix}, \\ F_{2,3}^{-(2)} &= -90\beta^{\text{eqv}} \begin{bmatrix} 1 & 2 \\ 4 & 6 \end{bmatrix} + 90\beta^{\text{eqv}} \begin{bmatrix} 2 & 1 \\ 4 & 6 \end{bmatrix} + 90\beta^{\text{eqv}} \begin{bmatrix} 2 & 1 \\ 6 & 4 \end{bmatrix} - 90\beta^{\text{eqv}} \begin{bmatrix} 3 & 0 \\ 6 & 4 \end{bmatrix} - \frac{5}{7}\zeta_3\beta^{\text{eqv}} \begin{bmatrix} 1 \\ 4 \end{bmatrix}, \\ F_{2,5}^{-(6)} &= -1890\beta^{\text{eqv}} \begin{bmatrix} 1 & 4 \\ 4 & 10 \end{bmatrix} - 1512\beta^{\text{eqv}} \begin{bmatrix} 2 & 3 \\ 4 & 10 \end{bmatrix} + 1890\beta^{\text{eqv}} \begin{bmatrix} 4 & 1 \\ 10 & 4 \end{bmatrix} + 1512\beta^{\text{eqv}} \begin{bmatrix} 5 & 0 \\ 10 & 4 \end{bmatrix}, \end{aligned} \quad (3.16)$$

and the analogous β^{eqv} -representations of any $F_{m,k}^{\pm(s)}$ with $m+k \leq 12$ can be found in a file in the supplementary material. Modular forms $\beta^{\text{eqv}} \begin{bmatrix} j_1 & j_2 \\ k_1 & k_2 \end{bmatrix}$ of non-zero weight $(0, k_1+k_2-2j_1-2j_2-4)$ occur in derivatives such as

$$\begin{aligned} \pi \nabla_\tau F_{2,3}^{+(3)} &= -\frac{45}{2}\beta^{\text{eqv}} \begin{bmatrix} 2 & 2 \\ 4 & 6 \end{bmatrix} - 15\beta^{\text{eqv}} \begin{bmatrix} 3 & 1 \\ 6 & 4 \end{bmatrix} - \frac{15}{2}\beta^{\text{eqv}} \begin{bmatrix} 4 & 0 \\ 6 & 4 \end{bmatrix}, \\ \frac{\pi \bar{\nabla}_\tau F_{2,3}^{+(3)}}{y^2} &= -240\beta^{\text{eqv}} \begin{bmatrix} 1 & 1 \\ 4 & 6 \end{bmatrix} - 120\beta^{\text{eqv}} \begin{bmatrix} 2 & 0 \\ 4 & 6 \end{bmatrix} - 360\beta^{\text{eqv}} \begin{bmatrix} 2 & 0 \\ 6 & 4 \end{bmatrix}, \end{aligned} \quad (3.17)$$

which follow from the β^{eqv} -representations of $F_{m,k}^{\pm(s)}$ via (3.5) and their Laplace equations.

As detailed in [44], some of the $F_{m,k}^{\pm(s)}$ with $m+k \geq 7$ and $s \geq 6$ contain iterated integrals of holomorphic cusp forms and therefore go beyond MGFs. These cases determine the cusp-form contributions β_Δ^{sv} in (3.2) and will be discussed in section 3.4 below, see in particular (3.32) below for a simple example.

We conclude this section with depth-three examples of MGFs,

$$\begin{aligned} \mathcal{C}^+ \begin{bmatrix} 2 & 2 & 1 & 1 \\ 2 & 2 & 1 & 1 \end{bmatrix} &= 216\beta^{\text{eqv}} \begin{bmatrix} 2 & 1 & 0 \\ 4 & 4 & 4 \end{bmatrix} + 840\beta^{\text{eqv}} \begin{bmatrix} 1 & 3 \\ 4 & 8 \end{bmatrix} - 252\beta^{\text{eqv}} \begin{bmatrix} 2 & 2 \\ 4 & 8 \end{bmatrix} + 840\beta^{\text{eqv}} \begin{bmatrix} 3 & 1 \\ 8 & 4 \end{bmatrix} - 252\beta^{\text{eqv}} \begin{bmatrix} 4 & 0 \\ 8 & 4 \end{bmatrix} \\ &\quad + 3600\beta^{\text{eqv}} \begin{bmatrix} 2 & 2 \\ 6 & 6 \end{bmatrix} - 3200\beta^{\text{eqv}} \begin{bmatrix} 3 & 1 \\ 6 & 6 \end{bmatrix} + 2100\beta^{\text{eqv}} \begin{bmatrix} 4 & 0 \\ 6 & 6 \end{bmatrix} + 3212\beta^{\text{eqv}} \begin{bmatrix} 5 \\ 12 \end{bmatrix}, \\ \mathcal{C}^+ \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} &= \left(\frac{47}{72} + 1814400 c_{446} \right) \zeta_7 - 3\zeta_5\beta^{\text{eqv}} \begin{bmatrix} 1 \\ 4 \end{bmatrix} - 1260\zeta_3\beta^{\text{eqv}} \begin{bmatrix} 3 \\ 8 \end{bmatrix} - 180\zeta_3\beta^{\text{eqv}} \begin{bmatrix} 2 & 0 \\ 4 & 4 \end{bmatrix} \\ &\quad + 360(150\beta^{\text{eqv}} \begin{bmatrix} 1 & 2 & 1 \\ 4 & 4 & 6 \end{bmatrix} + 150\beta^{\text{eqv}} \begin{bmatrix} 3 & 0 & 1 \\ 6 & 4 & 4 \end{bmatrix} - 90\beta^{\text{eqv}} \begin{bmatrix} 1 & 1 & 2 \\ 4 & 4 & 6 \end{bmatrix} - 90\beta^{\text{eqv}} \begin{bmatrix} 2 & 1 & 1 \\ 6 & 4 & 4 \end{bmatrix} \\ &\quad - 90\beta^{\text{eqv}} \begin{bmatrix} 1 & 2 & 1 \\ 4 & 6 & 4 \end{bmatrix} + 150\beta^{\text{eqv}} \begin{bmatrix} 1 & 3 & 0 \\ 4 & 6 & 4 \end{bmatrix} + 150\beta^{\text{eqv}} \begin{bmatrix} 2 & 1 & 1 \\ 4 & 6 & 4 \end{bmatrix} + 195\beta^{\text{eqv}} \begin{bmatrix} 2 & 0 & 2 \\ 4 & 4 & 6 \end{bmatrix} \\ &\quad + 195\beta^{\text{eqv}} \begin{bmatrix} 2 & 2 & 0 \\ 6 & 4 & 4 \end{bmatrix} + 15\beta^{\text{eqv}} \begin{bmatrix} 2 & 2 & 0 \\ 4 & 6 & 4 \end{bmatrix} - 330\beta^{\text{eqv}} \begin{bmatrix} 2 & 1 & 1 \\ 4 & 4 & 6 \end{bmatrix} - 330\beta^{\text{eqv}} \begin{bmatrix} 3 & 1 & 0 \\ 6 & 4 & 4 \end{bmatrix} \\ &\quad + 480\beta^{\text{eqv}} \begin{bmatrix} 2 & 2 & 0 \\ 4 & 4 & 6 \end{bmatrix} + 480\beta^{\text{eqv}} \begin{bmatrix} 4 & 0 & 0 \\ 6 & 4 & 4 \end{bmatrix} + 315\beta^{\text{eqv}} \begin{bmatrix} 2 & 3 \\ 6 & 8 \end{bmatrix} + 315\beta^{\text{eqv}} \begin{bmatrix} 3 & 2 \\ 8 & 6 \end{bmatrix} \\ &\quad - 1190\beta^{\text{eqv}} \begin{bmatrix} 3 & 2 \\ 8 & 6 \end{bmatrix} - 1190\beta^{\text{eqv}} \begin{bmatrix} 4 & 1 \\ 8 & 6 \end{bmatrix} + 2800\beta^{\text{eqv}} \begin{bmatrix} 4 & 1 \\ 6 & 8 \end{bmatrix} + 2800\beta^{\text{eqv}} \begin{bmatrix} 5 & 0 \\ 8 & 6 \end{bmatrix} \\ &\quad + 243\beta^{\text{eqv}} \begin{bmatrix} 4 & 1 \\ 10 & 4 \end{bmatrix} + 243\beta^{\text{eqv}} \begin{bmatrix} 1 & 4 \\ 4 & 10 \end{bmatrix} + 432\beta^{\text{eqv}} \begin{bmatrix} 5 & 0 \\ 10 & 4 \end{bmatrix} + 432\beta^{\text{eqv}} \begin{bmatrix} 2 & 3 \\ 4 & 10 \end{bmatrix} \\ &\quad + 3640\beta^{\text{eqv}} \begin{bmatrix} 6 \\ 14 \end{bmatrix}), \end{aligned} \quad (3.18)$$

where the former has been previously expressed in terms of iterated integrals [42, 65]. Moreover, the six-column MGF in (3.18) is sometimes denoted by $D_{5,1,1}$ in the literature

and provided the first example of an irreducible single-valued MZV beyond depth one in the expansion of MGFs around the cusp [29]. In our setting, the depth-three MZV $\zeta_{3,5,3}$ enters $\mathcal{C}^+[\frac{2}{2} \frac{1}{1} \frac{1}{1} \frac{1}{1} \frac{1}{1}]$ via $c^{\text{sv}}[\frac{2}{4} \frac{2}{4} \frac{4}{6}]$ in (3.10), and the role of rational free parameter c_{446} is explained below (3.11).

3.3 From Tsunogai’s derivation algebra to $\bar{\alpha}$

Apart from the constants c^{sv} and the cusp-form contributions $\overline{\beta_{\Delta}^{\text{sv}}}$ in the modular forms (3.3), we still need to supply the antiholomorphic T -invariants $\overline{\alpha[\dots; \tau]}$ (or their $\mathbb{Q}[y^{-1}]$ -linear combinations $\overline{\kappa[\dots; \tau]}$) entering the β^{sv} in (2.14). A variety of depth-two cases has been determined from the reality properties (2.25) of MGFs (or respective generating functions [42]) and those of the above solutions to inhomogeneous Laplace equations, $\overline{F_{m,k}^{\pm(s)}} = \pm F_{m,k}^{\pm(s)}$ [43, 44]: any $\overline{\alpha[\frac{j_1}{k_1} \frac{j_2}{k_2}; \tau]}$ is a linear combination of

$$\begin{aligned} \mathcal{E}_0(k, 0^p; \tau) &= \frac{(2\pi i)^{p+1-k}}{p!} \int_{\tau}^{i\infty} d\tau_1 (\tau - \tau_1)^p [\mathcal{G}_k(\tau_1) - 2\zeta_k] \\ &= -\frac{2}{(k-1)!} \sum_{m,n=1}^{\infty} \frac{q^{mn}}{m^{p-k+2} n^{p+1}}, \quad q = e^{2\pi i \tau}, \end{aligned} \tag{3.19}$$

with \mathbb{Q} -multiples of odd Riemann zeta values as coefficients. Modular T -invariance is attained through the subtraction of the zero mode $\mathcal{G}_k(\tau) = 2\zeta_k + O(q)$ in the integrand of (3.19) [66] and manifest from the q -series representation in the second line. The subtraction of the zero mode also makes the integral well-defined without the use of tangential-basepoint regularization. We note for future reference that the conjugates of these integrals can be rewritten as (with Bernoulli numbers B_k)

$$\overline{\mathcal{E}_0(k, 0^p; \tau)} = -\frac{B_k(-2\pi i \bar{\tau})^{p+1}}{k!(p+1)!} + \frac{1}{p!} \sum_{\ell=0}^{k-2-p} \frac{\binom{k-2-p}{\ell}}{(-4y)^\ell} \beta_- \left[\begin{matrix} p+\ell \\ k \end{matrix}; \tau \right], \tag{3.20}$$

when using the integrals β_- of the antiholomorphic kernels introduced in (2.15).

The examples of the $\overline{\alpha[\dots; \tau]}$ in the ancillary files of [43, 44] can be lined up with the following general formula at depth two,

$$\begin{aligned} \overline{\alpha \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} &= \overline{\alpha_{\text{easy}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} + \overline{\alpha_{\text{hard}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]}, \\ \overline{\alpha_{\text{easy}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} &= \frac{2\zeta_{k_1-1}}{k_1-1} \delta_{j_1, k_1-2} j_2! \overline{\mathcal{E}_0(k_2, 0^{j_2})} - \frac{2\zeta_{k_2-1}}{k_2-1} \delta_{j_2, k_2-2} j_1! \overline{\mathcal{E}_0(k_1, 0^{j_1})}. \end{aligned} \tag{3.21}$$

The second part $\overline{\alpha_{\text{hard}}}$ is the crucial hint to anticipate the connection between MGFs or β^{sv} and Brown’s EIEIs: the $\overline{\alpha_{\text{hard}}}$ are specified by a generating series

$$\begin{aligned} &\sum_{k_1, k_2=4}^{\infty} \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \frac{(k_1-1)(k_2-1)(-1)^{j_1+j_2}}{(k_1-j_1-2)!(k_2-j_2-2)!} \overline{\alpha_{\text{hard}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} \epsilon_{k_2}^{(k_2-j_2-2)} \epsilon_{k_1}^{(k_1-j_1-2)} \\ &= \sum_{m=1}^{\infty} 2\zeta_{2m+1} \sum_{k=4}^{\infty} \sum_{j=0}^{k-2} \frac{(k-1)(-1)^j}{(k-j-2)!} j! \overline{\mathcal{E}_0(k, 0^j)} [z_{2m+1}, \epsilon_k^{(k-j-2)}] \Big|_{\text{depth } 2} \end{aligned} \tag{3.22}$$

akin to (2.18), where we use the shorthand (2.20), and an explicit closed form of $\overline{\alpha_{\text{hard}}}$ derived from (3.22) can be found in appendix A.

The brackets in the second line of (3.22) involve derivations z_3, z_5, z_7, \dots dual to odd zeta values subject to $[z_{2m+1}, \epsilon_0] = 0$ that normalize² Tsunogai's derivation algebra: any $[z_{2m+1}, \epsilon_{k \neq 0}]$ in (3.22) is expressible in terms of nested commutators of two and more $\epsilon_{k_i}^{(j_i)}$ through a procedure described in [53] which relies on expressing the derivations in terms of elements of a free Lie algebra with two generators.

The ‘‘depth-two’’ contributions from $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$ are known in closed form, see [55, section 25],

$$[z_{2m-1}, \epsilon_{2n+2}]|_{\text{depth } 2} = \frac{(2n+2)! B_{2n+2m}}{(2n+2m-2)!(2n+2m)! B_{2n+2}} \sum_{\ell=0}^{2m-2} \frac{(-1)^\ell}{\ell!} (2n+\ell)! [\epsilon_{2m}^{(\ell)}, \epsilon_{2n+2m}^{(2m-2-\ell)}]. \quad (3.23)$$

The simplest examples of full $[z_{2m+1}, \epsilon_{k \neq 0}]$ -relations are

$$\begin{aligned} [z_3, \epsilon_4] &= \frac{1}{504} \left(-[\epsilon_4, \epsilon_6^{(2)}] + 3[\epsilon_4^{(1)}, \epsilon_6^{(1)}] - 6[\epsilon_4^{(2)}, \epsilon_6] \right), \\ [z_3, \epsilon_6] &= \frac{1}{1200} \left(-[\epsilon_4, \epsilon_8^{(2)}] + 5[\epsilon_4^{(1)}, \epsilon_8^{(1)}] - 15[\epsilon_4^{(2)}, \epsilon_8] + 63[\epsilon_4, [\epsilon_4^{(1)}, \epsilon_4]] \right), \\ [z_5, \epsilon_4] &= \frac{1}{604800} \left([\epsilon_6, \epsilon_8^{(4)}] - 3[\epsilon_6^{(1)}, \epsilon_8^{(3)}] + 6[\epsilon_6^{(2)}, \epsilon_8^{(2)}] - 10[\epsilon_6^{(3)}, \epsilon_8^{(1)}] + 15[\epsilon_6^{(4)}, \epsilon_8] \right. \\ &\quad + 105[\epsilon_4^{(1)}, [\epsilon_4^{(1)}, \epsilon_6^{(1)}]] - 1668[\epsilon_4^{(1)}, [\epsilon_4^{(2)}, \epsilon_6]] - 729[\epsilon_4^{(2)}, [\epsilon_4, \epsilon_6^{(1)}]] + 1458[\epsilon_4^{(2)}, [\epsilon_4^{(1)}, \epsilon_6]] \\ &\quad \left. + 35[\epsilon_4, [\epsilon_4, \epsilon_6^{(3)}]] - 313[\epsilon_4, [\epsilon_4^{(1)}, \epsilon_6^{(2)}]] + 834[\epsilon_4, [\epsilon_4^{(2)}, \epsilon_6^{(1)}]] + 208[\epsilon_4^{(1)}, [\epsilon_4, \epsilon_6^{(2)}]] \right), \end{aligned} \quad (3.24)$$

where the term $\sim [\epsilon_4, [\epsilon_4^{(1)}, \epsilon_4]]$ in the middle equation is the first instance of the higher-depth terms that are suppressed in (3.23). Combining (3.24) and (3.22) reproduces contributions such as [42]

$$\begin{aligned} \overline{\alpha_{\text{hard}}[{}^0_4 \ 2_6; \tau]} &= \frac{\zeta_3}{630} \overline{\mathcal{E}_0(4; \tau)}, \\ \overline{\alpha_{\text{hard}}[{}^2_4 \ 1_6; \tau]} &= \frac{\zeta_3}{210} \overline{\mathcal{E}_0(4, 0; \tau)}, \\ \overline{\alpha_{\text{hard}}[{}^0_4 \ 4_6; \tau]} &= \frac{2\zeta_3}{105} \overline{\mathcal{E}_0(4, 0, 0; \tau)}, \end{aligned} \quad (3.25)$$

or [43, 67]

$$\overline{\alpha_{\text{hard}}[{}^1_4 \ 3_8; \tau]} = -\frac{\zeta_3}{140} \overline{\mathcal{E}_0(6, 0, 0; \tau)}, \quad \overline{\alpha_{\text{hard}}[{}^2_6 \ 3_8; \tau]} = -\frac{\zeta_5}{98000} \overline{\mathcal{E}_0(4, 0; \tau)}. \quad (3.26)$$

Note that (3.23) readily implies that $\overline{\alpha_{\text{hard}}[{}^{j_1}_{k_1} \ j_2_{k_2}; \tau]}$ vanishes whenever $k_1 = k_2$. Any contribution of $\zeta_{2a-1} \beta^{\text{eqv}}[{}^j_w]$ to the β^{eqv} -representation of $F_{m,k}^{\pm(s)}$ (such as the term $-\frac{5}{7} \zeta_3 \beta^{\text{eqv}}[{}^1_4]$ in the expression (3.16) for $F_{2,3}^{-(2)}$) can be traced back to $\overline{\alpha_{\text{hard}}}$ and only occurs for $s = k - m + 1$.

²The normalizer, $N_{\mathfrak{g}}(S)$, of a subset S in a Lie algebra \mathfrak{g} is defined by $N_{\mathfrak{g}}(S) = \{z \in \mathfrak{g} \text{ s.t. } [z, x] \in S, \forall x \in S\}$.

In principle, one could use the commutator relations among ϵ_k in (2.21) to eliminate some of the terms $[\epsilon_6^{(j)}, \epsilon_8^{(4-j)}]$ in the expression (3.24) for $[z_5, \epsilon_4]$ in favor of $[\epsilon_4^{(j)}, \epsilon_{10}^{(4-j)}]$. The coefficients of $\epsilon_{k_1}^{(j_1)} \epsilon_{k_2}^{(j_2)}$ in the generating-series identity (3.22) are understood to be compared after importing the direct outcome of (3.23) for the commutators $[z_{2m+1}, \epsilon_k]$ and before inserting any relation among $[\epsilon_{k_1}, \epsilon_{k_2}]$ [49, 53, 62].³ With this convention, the $\overline{\alpha_{\text{hard}}}$ are individually well-defined by (3.22), see the closed formula in appendix A, which would not be the case when employing relations in Tsunogai's derivation algebra from the beginning. Beyond depth two, where we do not present a closed form analogous to (3.23), this convention will no longer fix all possible shifts of $[z_{2m+1}, \epsilon_{k \neq 0}]$ -relations by relations in Tsunogai's algebra (or ad_{ϵ_0} -actions thereon). Hence, additional criteria must be imposed to land on a canonical form for depth ≥ 3 contributions to the commutation relations.

3.4 Projecting out cusp forms

Holomorphic cusp forms $\Delta_{2s}(\tau)$ do not arise in the differential equations of MGFs [20, 26, 28] and their generating series [41]. Hence, iterated-integral representations of MGFs can only involve those combinations of β^{eqv} in (3.3) where the cusp-form contributions $\beta_{\Delta}^{\text{sv}}$ cancel. These cancellations can be conveniently implemented by dressing with Tsunogai's derivations

$$\begin{aligned}
 J^{\text{eqv}}(\{\epsilon_k\}; \tau) &= \sum_P \epsilon[P] \beta^{\text{eqv}}[P; \tau] \\
 &= 1 + \sum_{k=4}^{\infty} \sum_{j=0}^{k-2} \frac{(-1)^j (k-1)}{(k-2-j)!} \beta^{\text{eqv}} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right] \epsilon_k^{(k-j-2)} \\
 &\quad + \sum_{k_1=4}^{\infty} \sum_{k_2=4}^{\infty} \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \frac{(-1)^{j_1+j_2} (k_1-1)(k_2-1)}{(k_1-2-j_1)!(k_2-2-j_2)!} \beta^{\text{eqv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right] \epsilon_{k_2}^{(k_2-j_2-2)} \epsilon_{k_1}^{(k_1-j_1-2)} + \dots
 \end{aligned} \tag{3.27}$$

as in the generating series (2.18) of closed-string integrals over the torus. The words $\epsilon[P]$ in derivations ϵ_k are defined in (2.19) without committing to a matrix representation, and the ellipsis in the last line of (3.27) refers to $\beta^{\text{eqv}} \left[\begin{matrix} j_1 & \dots & j_\ell \\ k_1 & \dots & k_\ell \end{matrix} \right]$ of depth $\ell \geq 3$.

While all $\beta_{\Delta}^{\text{sv}} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right]$ at depth one and $\beta_{\Delta}^{\text{sv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]$ in (3.3) at $k_1+k_2 < 14$ vanish, their simplest non-trivial instances occur in the Laplace eigenfunctions $F_{m,k}^{\pm(s)}$ with $m+k \geq 7$ and $s \geq 6$ [43, 44] as well as their $\tau, \bar{\tau}$ derivatives. The results in the references translate into

$$\beta_{\Delta}^{\text{sv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right] = \sum_{\substack{\Delta_{2s} \text{ at} \\ 2s \leq k_1+k_2-2}} \xi_{k_1, k_2}^{\Delta_{2s}} A_{k_1, k_2, N}^{j_1, j_2} \beta^{\text{sv}} \left[\begin{matrix} j_1+j_2-N \\ \Delta_{2s}^{\pm} \end{matrix}; \tau \right], \tag{3.28}$$

where $N = \frac{1}{2}(k_1+k_2) - s - 1$, and the rational numbers $A_{k_1, k_2, N}^{j_1, j_2}$ are given by

$$A_{k_1, k_2, N}^{j_1, j_2} = \frac{1}{k_1! k_2!} \sum_{\ell=0}^N (-1)^\ell \binom{N}{\ell} \frac{j_1! (k_1-2-j_1)! j_2! (k_2-2-j_2)!}{(j_1-N+\ell)! (k_1-j_1-2-\ell)! (k_2-2-j_2-N+\ell)! (j_2-\ell)!}. \tag{3.29}$$

³It appears unnatural to rewrite the expressions (3.23) for the commutators $[z_{2m+1}, \epsilon_k]$ via relations in Tsunogai's derivation algebra: the relative factors $[\epsilon_6, \epsilon_8^{(4)}] - 3[\epsilon_6^{(1)}, \epsilon_8^{(3)}] + \dots$ in the expression (3.24) for $[z_5, \epsilon_4]$ are not reproduced by the binomials in the corollary $0 = \text{ad}_{\epsilon_0}^4([\epsilon_4, \epsilon_{10}] - 3[\epsilon_6, \epsilon_8]) = \sum_{j=0}^4 \binom{4}{j} ([\epsilon_4^{(j)}, \epsilon_{10}^{(4-j)}] - 3[\epsilon_6^{(j)}, \epsilon_8^{(4-j)}])$ of (2.21). The representation of $[z_5, \epsilon_4]$ in (3.24) is singled out by having no contribution of $[\epsilon_4^{(j)}, \epsilon_{10}^{(4-j)}]$, but it is not possible to eliminate all the $[\epsilon_6^{(j)}, \epsilon_8^{(4-j)}]$ with $j = 0, 1, 2, 3, 4$.

Moreover, we introduce the following delta-variant of the β^{sv} in (2.8) with $j = 0, 1, \dots, k-2$,

$$\beta^{\text{sv}} \left[\Delta_{\pm}^j; \tau \right] = (2\pi i)^{k-1} \left\{ \int_{\tau}^{i\infty} d\tau_1 \left(\frac{\tau - \tau_1}{4y} \right)^{k-2-j} (\bar{\tau} - \tau_1)^j \Delta_k(\tau_1) \right. \\ \left. \mp \int_{\bar{\tau}}^{-i\infty} d\bar{\tau}_1 \left(\frac{\tau - \bar{\tau}_1}{4y} \right)^{k-2-j} (\bar{\tau} - \bar{\tau}_1)^j \overline{\Delta_k(\tau_1)} \right\}. \quad (3.30)$$

The constants $\xi_{k_1, k_2}^{\Delta_{2s}}$ in (3.28) do not depend on j_1, j_2 and are expected to be transcendental, for instance [44]

$$\begin{aligned} (\xi_{4,10}^{\Delta_{12}}, \xi_{6,8}^{\Delta_{12}}) &= \left(-\frac{32}{45}, \frac{96}{175} \right) \frac{\Lambda(\Delta_{12}, 12)}{\Lambda(\Delta_{12}, 10)}, \\ (\xi_{4,12}^{\Delta_{12}}, \xi_{6,10}^{\Delta_{12}}, \xi_{8,8}^{\Delta_{12}}) &= \left(-\frac{576}{3455}, \frac{75}{691}, -\frac{64}{691} \right) \frac{\Lambda(\Delta_{12}, 13)}{\Lambda(\Delta_{12}, 11)}, \\ (\xi_{4,14}^{\Delta_{16}}, \xi_{6,12}^{\Delta_{16}}, \xi_{8,10}^{\Delta_{16}}) &= \left(-\frac{96}{35}, \frac{432}{385}, -\frac{32}{49} \right) \frac{\Lambda(\Delta_{16}, 16)}{\Lambda(\Delta_{16}, 14)}, \\ (\xi_{4,14}^{\Delta_{12}}, \xi_{6,12}^{\Delta_{12}}, \xi_{8,10}^{\Delta_{12}}) &= \left(-\frac{672}{44915}, \frac{8}{975}, -\frac{8}{1365} \right) \frac{\Lambda(\Delta_{12}, 14)}{\Lambda(\Delta_{12}, 10)}. \end{aligned} \quad (3.31)$$

As explained in the reference, the $\xi_{k_1, k_2}^{\Delta_{2s}}$ are ratios of L -values $\Lambda(\Delta_{2s}, t)$ outside and inside the critical strip $t \in (0, 2s)$ (with critical denominators $\Lambda(\Delta_{2s}, 2s-2)$ and $\Lambda(\Delta_{2s}, 2s-1)$ if $s + \frac{1}{2}(k_1 + k_2)$ is odd and even, respectively). The complete list of $\xi_{k_1, k_2}^{\Delta_{2s}}$ with $k_1 + k_2 \leq 24$ can be found in the supplementary material attached to this paper.

The simplest instance of integrals (3.30) over holomorphic cusp forms occurs in the modular invariant $F_{2,5}^{-(6)}(\tau)$, where the β^{eqv} -representation in (3.17) gives rise to

$$\begin{aligned} F_{2,5}^{-(6)}(\tau) |_{\Delta} &= 1890\beta_{\Delta}^{\text{sv}} \left[\frac{4}{10} \frac{1}{4}; \tau \right] - 1890\beta_{\Delta}^{\text{sv}} \left[\frac{1}{4} \frac{4}{10}; \tau \right] + 1512\beta_{\Delta}^{\text{sv}} \left[\frac{5}{10} \frac{0}{4}; \tau \right] - 1512\beta_{\Delta}^{\text{sv}} \left[\frac{2}{4} \frac{3}{10}; \tau \right] \\ &= \frac{\Lambda(\Delta_{12}, 12)}{18000\Lambda(\Delta_{12}, 10)} \beta^{\text{sv}} \left[\Delta_{\frac{12}{2}}^5; \tau \right], \end{aligned} \quad (3.32)$$

and the notation $|_{\Delta}$ on the left-hand side instructs us to suppress all Eisenstein integrals and depth-zero terms. More generally, the sign in the superscript of $F_{m,k}^{\pm(s)}$ matches that of the $\beta^{\text{sv}} \left[\Delta_{\pm}^j; \tau \right]$ in the iterated-integral representations of $F_{m,k}^{\pm(s)}$ and their modular derivatives. In particular, the $\beta^{\text{sv}} \left[\Delta_{\pm}^j; \tau \right]$ with the middle value $j = s-1$ correspond to the solutions $H_{\Delta_{2s}}^{\pm}$ of homogeneous Laplace equations⁴ [44],

$$\beta^{\text{sv}} \left[\Delta_{\pm}^{s-1}; \tau \right] = -2(s-1)! H_{\Delta_{2s}}^{\pm}(\tau), \quad (3.33)$$

⁴Larger (smaller) values of j correspond to the $(j-s+1)^{\text{th}}$ τ -derivative and $(s-1-j)^{\text{th}}$ $\bar{\tau}$ -derivative of $H_{\Delta_{2s}}^{\pm}$, respectively, where $\nabla_{\tau} = 2i(\text{Im } \tau)^2 \partial_{\tau}$:

$$\begin{aligned} \beta^{\text{sv}} \left[\Delta_{\pm}^{s-1+m}; \tau \right] &= -2(-4)^m (s-1-m)! (\pi \nabla_{\tau})^m H_{\Delta_{2s}}^{\pm}(\tau), \\ \beta^{\text{sv}} \left[\Delta_{\pm}^{s-1-m}; \tau \right] &= \frac{-2(s-1-m)! (\pi \bar{\nabla}_{\tau})^m H_{\Delta_{2s}}^{\pm}(\tau)}{(-4)^m y^{2m}}. \end{aligned}$$

whose appearance in the $\mathbb{F}_{m,k}^{\pm(s)}$ is discussed in the reference. Note that the shuffles (3.13) relate $\beta_{\Delta}^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}; \tau \right] = -\beta_{\Delta}^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]$ which together with the parity property $A_{k_2, k_1, N}^{j_2, j_1} = (-1)^N A_{k_1, k_2, N}^{j_1, j_2}$ of (3.29) implies that

$$\xi_{k_2, k_1}^{\Delta_{2s}} = (-1)^{s+\frac{1}{2}(k_1+k_2)} \xi_{k_1, k_2}^{\Delta_{2s}}. \tag{3.34}$$

Starting from depth three, the $\beta_{\Delta}^{\text{sv}}$ will generically involve both (3.30) and double integrals that combine kernels G_k and Δ_{2s} and will be investigated in [45].

All the $\beta_{\Delta_{\pm}^j}^{\text{sv}} \left[\begin{smallmatrix} j \\ \Delta_{\pm}^j \end{smallmatrix}; \tau \right]$ and their higher-depth generalizations cancel from the generating series (3.27) since their coefficients vanish by the relations in the derivation algebra [49, 53, 62]: the overall coefficient in (3.27) of $\frac{\Lambda(\Delta_{12}, 12)}{\Lambda(\Delta_{12}, 10)} \beta_{\Delta_{12}^-}^{\text{sv}} \left[\begin{smallmatrix} j \\ \Delta_{12}^- \end{smallmatrix}; \tau \right]$ is, for instance, proportional to

$$\text{ad}_{\epsilon_0}^{10-j}([\epsilon_4, \epsilon_{10}] - 3[\epsilon_6, \epsilon_8]) = 0, \tag{3.35}$$

and more general coefficients of $H_{\Delta_{2s}^{\pm}}$ in the series (3.27) are described in section 4 of [44]. By the depth-three terms $[\epsilon_4, [\epsilon_4, \epsilon_8]]$ and $[\epsilon_6, [\epsilon_6, \epsilon_4]]$ in the last relation of (2.21), the cancellation of $\frac{\Lambda(\Delta_{12}, 13)}{\Lambda(\Delta_{12}, 11)} \beta_{\Delta_{12}^+}^{\text{sv}} \left[\begin{smallmatrix} j \\ \Delta_{12}^+ \end{smallmatrix}; \tau \right]$ also hinges on contributions from $\beta_{\Delta}^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 4 & 8 \end{smallmatrix}; \tau \right]$ and $\beta_{\Delta}^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 6 & 6 & 4 \end{smallmatrix}; \tau \right]$, see [45] for details.

Given the cancellation of cusp-form contributions, the differential equation of the generating series (3.27) is determined by the terms in the τ -derivatives of β^{eqv} displayed in (3.5):

$$-2\pi i(\tau - \bar{\tau})^2 \partial_{\tau} J^{\text{eqv}}(\{\epsilon_k\}; \tau) = \text{ad}_{\epsilon_0} J^{\text{eqv}}(\{\epsilon_k\}; \tau) + \sum_{m=4}^{\infty} (m-1)(\tau - \bar{\tau})^m G_m(\tau) \epsilon_m J^{\text{eqv}}(\{\epsilon_k\}; \tau). \tag{3.36}$$

Up to convention-dependent powers of $\tau - \bar{\tau}$ and normalization factors of the holomorphic Eisenstein series, this matches the holomorphic derivative of Brown’s generating series J^{eqv} in section 8.2 of [37]. In comparison to the differential equation of the generating series $Y_{\bar{\eta}}^{\tau}$ in section 2.4 of [42], left-action of the operator $R_{\bar{\eta}}(\epsilon_0)$ is replaced by the adjoint action ad_{ϵ_0} in (3.36) since ∂_{τ} no longer acts on the exponential in (2.18).

4 Connection with equivariant iterated Eisenstein integrals

In this section, we relate the modular forms β^{eqv} introduced in the preceding section to Brown’s EIEIs by equating certain generating series.

4.1 Matching β^{eqv} with Brown’s construction

We begin by describing an alternative way to assemble the generating series (3.27) of the modular forms β^{eqv} : instead of combining the holomorphic and anti-holomorphic iterated Eisenstein integrals β_{\pm} into the β^{sv} as in (2.14), we organize them into separate generating series

$$J_{\pm}(\{\epsilon_k\}; \tau) = \sum_P \epsilon[P] \beta_{\pm}[P; \tau], \tag{4.1}$$

see (2.15) for β_{\pm} and (2.19) for the words $\epsilon[P]$ in ϵ_k . The sums in (4.1) and below over P are again over all words $P = \begin{smallmatrix} j_1 & \dots & j_{\ell} \\ k_1 & \dots & k_{\ell} \end{smallmatrix}$ of length $\ell \geq 0$ with $k_i \geq 4$ even and $0 \leq j_i \leq k_i - 2$.

The central result of this work is that the modular forms β^{eqv} constructed in (3.3) can be alternatively generated via

$$J^{\text{eqv}}(\{\epsilon_k\}; \tau) = J_+(\{\epsilon_k\}; \tau) B^{\text{sv}}(\{\epsilon_k\}; \tau) \phi^{\text{sv}}(\widetilde{J}_-(\{\epsilon_k\}; \tau)). \quad (4.2)$$

The ingredients B^{sv} and ϕ^{sv} follow Brown’s construction in [37], see section 4.1.1 for the series B^{sv} in MZVs, and the change of alphabet ϕ^{sv} will be made fully explicit in section 4.1.2 below. The tilde of $\widetilde{J}_-(\{\epsilon_k\}; \tau)$ instructs us to reverse the words $\epsilon_{k_1}^{(j_1)} \dots \epsilon_{k_\ell}^{(j_\ell)} \rightarrow \epsilon_{k_\ell}^{(j_\ell)} \dots \epsilon_{k_1}^{(j_1)}$ without additional j_i -dependent minus-signs that one may have expected from the $\text{ad}_{\epsilon_0^-}$ -action. Note that the change of alphabet ϕ^{sv} is performed *after* reversal of the word in $\epsilon_{k_i}^{(j_i)}$, and it would lead to an incorrect expression if the reversal is applied to the image of ϕ^{sv} .

The series J^{eqv} with the modular transformation $\epsilon_k \rightarrow (c\bar{\tau}+d)^{k-2}\epsilon_k$ of its bookkeeping variables under $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z})$ [36, 37] is modular invariant and referred to as generating EIEIs. As emphasized before, by slight abuse of notation, we allude to equivariance in the superscript of the component integrals β^{eqv} in (3.27) even though they transform as modular forms according to (3.6).

4.1.1 The generating series B^{sv} in single-valued MZVs

The series B^{sv} of single-valued MZVs in (4.2) is claimed to be constructed from the constants c^{sv} in the conversion (3.3) from β^{sv} to β^{eqv} . However, the rational dependence of the d^{sv} on $y = \pi \text{Im } \tau$ in (3.4) needs to be augmented by additional powers of $\bar{\tau}$ in the numerator

$$b^{\text{sv}} \left[\begin{matrix} \dots & j_i & \dots \\ \dots & k_i & \dots \end{matrix}; \tau \right] = \sum_{p_i=0}^{k_i-2-j_i} \sum_{\ell_i=0}^{j_i+p_i} \binom{k_i-2-j_i}{p_i} \binom{j_i+p_i}{\ell_i} \frac{(-2\pi i \bar{\tau})^{\ell_i}}{(4y)^{p_i}} c^{\text{sv}} \left[\begin{matrix} \dots & j_i-\ell_i+p_i & \dots \\ \dots & k_i & \dots \end{matrix} \right], \quad (4.3)$$

where we have one double-sum over p_i, ℓ_i per column. The rational dependence on τ and $\bar{\tau}$ can be understood from the transformation between the coefficient c^{sv} of $Y_i^{j_i} X_i^{k_i-j_i-2}$ and b^{sv} of $(X_i-\tau Y_i)^{j_i} (X_i-\bar{\tau} Y_i)^{k_i-j_i-2}$, similar to the transformation of integration kernels in (2.13).

At depth one, the additional $\bar{\tau}$ -dependence still cancels by the simple form of $c^{\text{sv}} \begin{bmatrix} j \\ k \end{bmatrix}$ in (3.7),

$$b^{\text{sv}} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right] = -\frac{2\zeta_{k-1}}{(k-1)(4y)^{k-2-j}}, \quad (4.4)$$

but already the simplest depth-two examples depend non-trivially on $\bar{\tau}$ and therefore vary under the modular T -transformation,

$$\begin{aligned} b^{\text{sv}} \left[\begin{matrix} 1 & 0 \\ 4 & 4 \end{matrix}; \tau \right] &= \frac{\zeta_3}{2160} - \frac{i\bar{\tau}\pi\zeta_3}{2160y} - \frac{\bar{\tau}^2\pi^2\zeta_3}{8640y^2} + \frac{\zeta_3^2}{288y^3} - \frac{5\zeta_5}{1728y^2}, \\ b^{\text{sv}} \left[\begin{matrix} 2 & 0 \\ 4 & 4 \end{matrix}; \tau \right] &= -\frac{i\bar{\tau}\pi\zeta_3}{540} - \frac{\bar{\tau}^2\pi^2\zeta_3}{1080y} + \frac{\zeta_3^2}{72y^2} - \frac{5\zeta_5}{216y}, \\ b^{\text{sv}} \left[\begin{matrix} 2 & 1 \\ 4 & 4 \end{matrix}; \tau \right] &= \frac{\bar{\tau}^2\pi^2\zeta_3}{540} + \frac{\zeta_3^2}{18y} + \frac{5\zeta_5}{108}. \end{aligned} \quad (4.5)$$

The alternative expression (4.2) for J^{eqv} is then built from the following generating series of b^{sv} :

$$B^{\text{sv}}(\{\epsilon_k\}; \tau) = \sum_P \epsilon[P] b^{\text{sv}}[P; \tau]. \quad (4.6)$$

4.1.2 The change of alphabet

The change of alphabet $\epsilon_k \rightarrow \phi^{\text{sv}}(\epsilon_k)$ in (4.2) acts on the series $\widetilde{\mathcal{J}}_-$ of antiholomorphic iterated Eisenstein integrals in (4.1) and maps each derivation to an infinite series in single-valued MZVs and nested commutators of $\epsilon_k^{(j)}$ [37]. Theorem 7.2 in [37] implicitly determines B^{sv} and ϕ^{sv} in terms of multiple modular values. The map ϕ^{sv} is an automorphism of the universal enveloping algebra of Tsunogai’s derivations, and we find its explicit form on single derivations to be given by

$$\phi^{\text{sv}}(\epsilon_0) = \epsilon_0, \quad \phi^{\text{sv}}(\epsilon_k) = \mathbb{M}^{\text{sv}} \epsilon_k (\mathbb{M}^{\text{sv}})^{-1}, \quad k \geq 4 \tag{4.7}$$

with the following group-like element:

$$\begin{aligned} \mathbb{M}^{\text{sv}} &= \sum_{\ell=0}^{\infty} \sum_{\substack{i_1, i_2, \dots, i_\ell \\ \in 2\mathbb{N}+1}} z_{i_1} z_{i_2} \dots z_{i_\ell} \rho^{-1}(\text{sv}(f_{i_1} f_{i_2} \dots f_{i_\ell})) \\ &= 1 + \sum_{i_1 \in 2\mathbb{N}+1} z_{i_1} \rho^{-1}(\text{sv}(f_{i_1})) + \sum_{i_1, i_2 \in 2\mathbb{N}+1} z_{i_1} z_{i_2} \rho^{-1}(\text{sv}(f_{i_1} f_{i_2})) + \dots \end{aligned} \tag{4.8}$$

The dependence on the derivations z_3, z_5, \dots discussed around (3.22) and (3.23) will not be displayed in the notation for \mathbb{M}^{sv} . Moreover, we use the f -alphabet description of (motivic) MZVs [68]⁵ with one non-commutative generator f_i for each $i \in 2\mathbb{N}+1$. The isomorphism ρ mapping MZVs to the f -alphabet

$$\begin{aligned} \rho(\zeta_i) &= f_i, \quad \rho(\zeta_i \zeta_j) = f_i \sqcup f_j = f_i f_j + f_j f_i, \quad i, j \in 2\mathbb{N}+1, \\ \rho(\zeta_{3,5}) &= -5 f_3 f_5, \quad \rho(\zeta_{3,5,3}) = -5 f_3 f_5 f_3 + \frac{299}{2} f_{11}, \\ \rho(\zeta_{3,5,3}^{\text{sv}}) &= -20(f_3 f_5 f_3 + f_5 f_3 f_3) + 299 f_{11} = \text{sv}\left(-5 f_3 f_5 f_3 + \frac{299}{2} f_{11}\right) \end{aligned} \tag{4.9}$$

is invertible and often denoted by ϕ instead of ρ in the mathematics and physics literature (see [1, 68] for examples beyond depth one).

In (4.9), we have given an example of the single-valued map in the f -alphabet. It takes the following simple form in the general case [63, 64]

$$\text{sv}(f_2^N f_{i_1} f_{i_2} \dots f_{i_\ell}) = \delta_{N,0} \sum_{j=0}^{\ell} f_{i_j} \dots f_{i_2} f_{i_1} \sqcup f_{i_{j+1}} f_{i_{j+2}} \dots f_{i_\ell}, \tag{4.10}$$

such that the depth-one and depth-two contributions to the change of alphabet (4.7) reduce to odd Riemann zeta values by $\text{sv}(f_i) = 2f_i$ and $\text{sv}(f_i f_j) = 2f_i \sqcup f_j = 2(f_i f_j + f_j f_i)$,

$$\phi^{\text{sv}}(\epsilon_k) = \epsilon_k + 2 \sum_{i_1 \in 2\mathbb{N}+1} \zeta_{i_1}[z_{i_1}, \epsilon_k] + 2 \sum_{i_1, i_2 \in 2\mathbb{N}+1} \zeta_{i_1} \zeta_{i_2}[z_{i_1}, [z_{i_2}, \epsilon_k]] + \dots \tag{4.11}$$

Also, at higher depth, each term boils down to nested brackets of $\epsilon_{k_i}^{(j_i)}$ since the z_3, z_5, \dots normalize the derivation algebra, see e.g. (3.24). The all-depth expression for the adjoint

⁵Both the f -alphabet and the single-valued map are only well-defined in the context of motivic MZVs whose elaborate definition can for instance be found in [69, 70].

action in (4.7) yields an infinite series of nested commutators

$$\phi^{\text{sv}}(\epsilon_k) = \sum_{\ell=0}^{\infty} \sum_{\substack{i_1, i_2, \dots, i_\ell \\ \in 2^{\mathbb{N}+1}}} [z_{i_1}, [z_{i_2}, \dots, [z_{i_{\ell-1}}, [z_{i_\ell}, \epsilon_k]] \dots]] \rho^{-1}(\text{sv}(f_{i_1} f_{i_2} \dots f_{i_\ell})), \quad (4.12)$$

which is implicit in Brown’s work [35, 37]. The action of ϕ^{sv} on higher-depth expressions in the ϵ_k derivations can be deduced from (4.12) via $\phi^{\text{sv}}(\epsilon_{k_1}^{(j_1)} \epsilon_{k_2}^{(j_2)} \dots) = (\text{ad}_{\epsilon_0}^{j_1} \phi^{\text{sv}}(\epsilon_{k_1})) (\text{ad}_{\epsilon_0}^{j_2} \phi^{\text{sv}}(\epsilon_{k_2})) \dots$ as can be seen from the conjugation action in (4.7). In the context of the series J^{eqv} in (3.27), conjugation (4.7) of the individual ϵ_k can be converted to the overall adjoint action

$$\phi^{\text{sv}}(\widetilde{J}_-(\{\epsilon_k\}; \tau)) = \mathbb{M}^{\text{sv}} \widetilde{J}_-(\{\epsilon_k\}; \tau) (\mathbb{M}^{\text{sv}})^{-1}. \quad (4.13)$$

Based on the ideas of [53], we have determined the commutators $[z_3, \epsilon_{k \leq 14}]$ and $[z_5, \epsilon_{k \leq 10}]$ and appended them in a file in the supplementary material attached to this paper. In this way, one can extract the contributions of ϕ^{sv} to all the $\beta^{\text{eqv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix} \right]$ with $k_1 + k_2 + k_3 \leq 16$ from (4.2).

Note that the analogue of $B^{\text{sv}}, \phi^{\text{sv}}$ described in Theorem 7.2 of [37]⁶ is only well-defined up to $B^{\text{sv}} \rightarrow B^{\text{sv}} a^{-1}$ and $\phi^{\text{sv}}(\widetilde{J}_-) \rightarrow a \phi^{\text{sv}}(\widetilde{J}_-) a^{-1}$ for some series a in $\epsilon_k^{(j)}$ whose coefficients are \mathbb{Q} -linear combinations of single-valued MZVs. Such redefinitions amount to right-multiplication of the series J^{eqv} in (4.2) by a^{-1} . One can view our realization (4.7) or (4.12) of ϕ^{sv} as fixing a particular “gauge-choice” of the series a , and it would be interesting to compare it with alternative choices. The one-parameter freedom of shifting certain $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 4 & 6 \end{smallmatrix} \right]$ and $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 6 & 6 \end{smallmatrix} \right]$ by ζ_7 and $\zeta_3 \zeta_5$ — see the discussion below (3.11) — corresponds to leading-depth contributions of schematic form $a = 1 + \zeta_7 [\epsilon_4^{(j_1)}, [\epsilon_4^{(j_2)}, \epsilon_6^{(j_3)}]] + \zeta_3 \zeta_5 [\epsilon_6^{(j_1)}, [\epsilon_6^{(j_2)}, \epsilon_4^{(j_3)}]] + \dots$ with $j_1 + j_2 + j_3 = 4$ and $j'_1 + j'_2 + j'_3 = 5$, respectively. This freedom should get fixed once we impose all β^{eqv} at depth four to arise from the change of alphabet ϕ^{sv} in the form (4.12): it requires at least one unit of depth from \widetilde{J}_- to distinguish $\phi^{\text{sv}}(\widetilde{J}_-)$ from $a \phi^{\text{sv}}(\widetilde{J}_-) a^{-1}$, so the departure of $a \phi^{\text{sv}}(\widetilde{J}_-) a^{-1}$ from (4.12) with the above depth-three contribution to a is at least fourth order in $\epsilon_k^{(j)}$. The reason why the discussion of a becomes more pressing at depth three is discussed in section 4.3.3.

Moreover, derivations z_i at $i \geq 11$ are only well defined up to nested commutators of $z_{i_1} z_{i_2} \dots$ with $i_1 + i_2 + \dots = i$, which, for instance, leaves an ambiguity of adding $[z_3, [z_5, z_3]]$ to z_{11} . This reflects the fact that the isomorphism ρ to the f -alphabet is non-canonical, e.g. the choice in (4.9) sets the coefficient of f_{11} in $\rho(\zeta_{3,3,5})$ to zero by convention. For a given choice of setting up the f -alphabet, there is a preferred scheme of fixing the ambiguity of $z_{i \geq 11}$, e.g. a specific representative of z_{11} adapted to having vanishing coefficient of f_{11} in $\rho(\zeta_{3,3,5})$.⁷ One then arrives at the same change of alphabet ϕ^{sv} for any choice of f -alphabet upon mapping back to (motivic) MZVs via ρ^{-1} in (4.12).

⁶The series b^{sv} in Brown’s work [37] corresponds to the inverse of B^{sv} defined in (4.6).

⁷More generally, the ρ -images of MZVs at weights $w \leq 16$ in [1] are taken to have a vanishing coefficients of f_w for each element of the bases in the datamine [71] (where $f_{2k} = \frac{\zeta_{2k}}{\binom{2k}{2}} f_2^k$ for even weight). As a result, the ρ -images of the weight-thirteen c^{sv} in (3.10) are computed from

$$\begin{aligned} \rho(\zeta_{5,3,5}) &= -60 f_3 f_5 f_5 - 5 f_5 f_3 f_5 + \frac{24}{35} f_2^4 f_5 + \frac{1003}{2} f_{13}, \\ \rho(\zeta_{3,7,3}) &= -66 f_3 f_5 f_5 - 6 f_5 f_3 f_5 - 6 f_5 f_5 f_3 - 14 f_3 f_7 f_3 + \frac{144}{175} f_2^4 f_5 + 716 f_{13}, \end{aligned}$$

which follow from the absence of f_{13} in the basis elements $\rho(\zeta_{3,5,5})$ and $\rho(\zeta_{3,3,7})$ [1, 71].

As will be detailed in future work, a conjugation formula similar to (4.7) applies to the letters in the generating series of antiholomorphic genus-zero polylogarithms that enter Brown's construction of single-valued polylogarithms in one variable [38].

4.1.3 Extracting components

By extracting the coefficients of $\epsilon[P]$ in (4.2), one can read off components

$$\beta^{\text{eqv}}[P; \tau] = \beta_{\Delta}^{\text{sv}}[P; \tau] + \sum_{P=XYZ} \beta_{-}^{\phi}[X^t; \tau] b^{\text{sv}}[Y; \tau] \beta_{+}[Z; \tau], \quad (4.14)$$

where the cusp-form contributions $\beta_{\Delta}^{\text{sv}}[P; \tau]$ are projected out from J^{eqv} by the relations among the ϵ_k , see section 3.4. We employ the shorthand

$$\beta_{-}^{\phi}[P^t; \tau] = \phi^{\text{sv}}(\widetilde{\mathcal{J}}_{-}(\{\epsilon_k\}; \tau)) \Big|_{\epsilon[P]} \quad (4.15)$$

for the iterated integrals of antiholomorphic Eisenstein series deformed by the change of alphabet in (4.12). Since any term in $[z_m, \epsilon_k]$ involves at least two letters $\epsilon_{k_i}^{(j_i)}$ and no instance of $\epsilon_{k_1}^{(j_1)} \epsilon_{k_2}^{(j_2)}$ with $k_1 = k_2$, we have

$$\beta_{-}^{\phi} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right] = \beta_{-} \left[\begin{matrix} j \\ k \end{matrix}; \tau \right], \quad \beta_{-}^{\phi} \left[\begin{matrix} j_1 & j_2 \\ k & k \end{matrix}; \tau \right] = \beta_{-} \left[\begin{matrix} j_1 & j_2 \\ k & k \end{matrix}; \tau \right]. \quad (4.16)$$

Hence, the simplest non-trivial corrections

$$\delta_{\phi} \beta_{-} \left[\begin{matrix} j_1 & \dots & j_{\ell} \\ k_1 & \dots & k_{\ell} \end{matrix}; \tau \right] = \beta_{-}^{\phi} \left[\begin{matrix} j_1 & \dots & j_{\ell} \\ k_1 & \dots & k_{\ell} \end{matrix}; \tau \right] - \beta_{-} \left[\begin{matrix} j_1 & \dots & j_{\ell} \\ k_1 & \dots & k_{\ell} \end{matrix}; \tau \right] \quad (4.17)$$

via ϕ^{sv} occur at depth two with $k_1 \neq k_2$, where the structure of (3.23) implies that $\delta_{\phi} \beta_{-} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} \right] = -\delta_{\phi} \beta_{-} \left[\begin{matrix} j_2 & j_1 \\ k_2 & k_1 \end{matrix} \right]$ are products of odd zeta values with $\beta_{-} \left[\begin{matrix} j \\ k \end{matrix} \right]$ of depth one. As one can anticipate from the examples

$$\begin{aligned} \delta_{\phi} \beta_{-} \left[\begin{matrix} 0 & 2 \\ 6 & 4 \end{matrix}; \tau \right] &= \frac{\zeta_3}{105} \beta_{-} \left[\begin{matrix} 0 \\ 4 \end{matrix}; \tau \right], \\ \delta_{\phi} \beta_{-} \left[\begin{matrix} 3 & 2 \\ 8 & 4 \end{matrix}; \tau \right] &= \frac{\zeta_3}{420} \beta_{-} \left[\begin{matrix} 3 \\ 6 \end{matrix}; \tau \right], \\ \delta_{\phi} \beta_{-} \left[\begin{matrix} 3 & 2 \\ 8 & 6 \end{matrix}; \tau \right] &= -\frac{\zeta_5}{98000} \beta_{-} \left[\begin{matrix} 1 \\ 4 \end{matrix}; \tau \right], \end{aligned} \quad (4.18)$$

as well as

$$\begin{aligned} \delta_{\phi} \beta_{-} \left[\begin{matrix} 1 & 2 & 2 \\ 4 & 4 & 4 \end{matrix}; \tau \right] &= \frac{7\zeta_3}{360} \beta_{-} \left[\begin{matrix} 4 \\ 6 \end{matrix}; \tau \right], \\ \delta_{\phi} \beta_{-} \left[\begin{matrix} 2 & 0 & 1 \\ 6 & 4 & 4 \end{matrix}; \tau \right] &= \frac{13\zeta_5}{141750} \beta_{-} \left[\begin{matrix} 0 \\ 4 \end{matrix}; \tau \right] - \frac{\zeta_3}{40} \beta_{-} \left[\begin{matrix} 2 \\ 8 \end{matrix}; \tau \right] + \frac{\zeta_3}{630} \beta_{-} \left[\begin{matrix} 0 & 1 \\ 4 & 4 \end{matrix}; \tau \right], \\ \delta_{\phi} \beta_{-} \left[\begin{matrix} 3 & 1 & 0 \\ 8 & 4 & 4 \end{matrix}; \tau \right] &= -\frac{\zeta_3^2}{352800} \beta_{-} \left[\begin{matrix} 0 \\ 4 \end{matrix}; \tau \right] - \frac{\zeta_5}{6048} \beta_{-} \left[\begin{matrix} 1 \\ 6 \end{matrix}; \tau \right] + \frac{33\zeta_3}{1750} \beta_{-} \left[\begin{matrix} 3 \\ 10 \end{matrix}; \tau \right] - \frac{\zeta_3}{280} \beta_{-} \left[\begin{matrix} 2 & 0 \\ 6 & 4 \end{matrix}; \tau \right], \end{aligned} \quad (4.19)$$

the ϕ^{sv} -corrections (4.17) to β_{-} of depth ℓ comprise iterated Eisenstein integrals of depth $\leq \ell-1$, and their coefficients are single-valued MZVs with one to $\ell-1$ letters in the f -alphabet. The simplest MGF that receives ϕ^{sv} -corrections is the non-holomorphic cusp form $\text{Im } \mathcal{C}^+ \left[\begin{matrix} 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 3 \end{matrix} \right]$ in (3.15). The real MGFs $\mathcal{C}^+ \left[\begin{matrix} a & b & c \\ 1 & a & b & c \end{matrix} \right]$ at $a+b+c \leq 6$ and $\mathcal{C}^+ \left[\begin{matrix} 2 & 2 & 1 & 1 \\ 2 & 2 & 1 & 1 \end{matrix} \right]$ with

iterated-integral representations in [42, 65] and (3.18) are unaffected by ϕ^{sv} , that is why cuspidal MGFs pioneered in [72] and further investigated in [42, 58] are essential case studies of the change of alphabet.

Note that the depth-two examples in (4.18) can be lined up with a closed formula

$$\delta_\phi \beta_- \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} \right] = \begin{cases} \frac{2(-1)^{j_1} \zeta_{k_1-1} (k_2-k_1+1)! (k_2-k_1+2)! j_2! (k_2-j_2-2)! B_{k_2}}{(k_1-1)k_2!(k_2-1)!(k_2-j_1-j_2-2)!(j_1+j_2-k_1+2)! B_{k_2-k_1+2}} \beta_- \left[\begin{matrix} j_1+j_2-k_1+2 \\ k_2-k_1+2 \end{matrix} \right] : k_1 < k_2, \\ -\frac{2(-1)^{j_2} \zeta_{k_2-1} (k_1-k_2+1)! (k_1-k_2+2)! j_1! (k_1-j_1-2)! B_{k_1}}{(k_2-1)k_1!(k_1-1)!(k_1-j_1-j_2-2)!(j_1+j_2-k_2+2)! B_{k_1-k_2+2}} \beta_- \left[\begin{matrix} j_1+j_2-k_2+2 \\ k_1-k_2+2 \end{matrix} \right] : k_1 > k_2, \\ 0 : k_1 = k_2, \end{cases} \quad (4.20)$$

which is equivalent to (4.49) below and the results of appendix A.

Since ϕ^{sv} does not contribute at depth one, the simplest examples of the β^{eqv} in the new description (4.14) read

$$\begin{aligned} \beta^{\text{eqv}} \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right] &= \beta_- \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right] + b^{\text{sv}} \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right] + \beta_+ \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right], \\ \beta^{\text{eqv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} \right] &= \beta_\Delta^{\text{sv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} \right] + \beta_+ \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} \right] + b^{\text{sv}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} \right] + \beta_- \left[\begin{matrix} j_2 & j_1 \\ k_2 & k_1 \end{matrix} \right] + \delta_\phi \beta_- \left[\begin{matrix} j_2 & j_1 \\ k_2 & k_1 \end{matrix} \right] \\ &\quad + b^{\text{sv}} \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right] \beta_+ \left[\begin{matrix} j_2 \\ k_2 \end{matrix} \right] + \beta_- \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right] b^{\text{sv}} \left[\begin{matrix} j_2 \\ k_2 \end{matrix} \right] + \beta_- \left[\begin{matrix} j_1 \\ k_1 \end{matrix} \right] \beta_+ \left[\begin{matrix} j_2 \\ k_2 \end{matrix} \right], \end{aligned} \quad (4.21)$$

see (3.2) for the earlier description in terms of β^{sv} . We have checked up to $k_1+k_2 = 24$ at depth two and $k_1+k_2+k_3 = 16$ at depth three that the expansions of (4.2) and (3.27) in terms of $\epsilon_{k_i}^{(j_i)}$ match after iteratively using the commutation relations $[z_m, \epsilon_k]$ in (3.24) and the supplementary material.

The main conjecture of this work is that the two constructions (4.2) and (3.27) of the generating series J^{eqv} agree to all orders in $\epsilon_{k_i}^{(j_i)}$. This conjecture implies that all MGFs — i.e. modular combinations of β^{sv} — are contained in the components of Brown’s EIEIs generated by (4.2). Further corollaries of this conjecture include the shuffle relations (3.13) of the building blocks $\beta^{\text{sv}}, c^{\text{sv}}$ of MGFs and the exclusive appearance of single-valued MZVs in the expansion of MGFs around the cusp as firstly proposed in [17, 29].

4.1.4 c^{sv} in the f -alphabet

The f -alphabet also reveals all-order properties of the single-valued MZVs in $c^{\text{sv}} \left[\begin{matrix} j_1 & \dots & j_\ell \\ k_1 & \dots & k_\ell \end{matrix} \right]$ that determine the components (4.3) of the series B^{sv} in (4.2): the results at depth ≤ 3 in section 3.1 and the supplementary material suggest that their instances at $j_i = k_i - 2$ obey a simple formula

$$\rho \left(c^{\text{sv}} \left[\begin{matrix} k_1-2 & k_2-2 & \dots & k_\ell-2 \\ k_1 & k_2 & \dots & k_\ell \end{matrix} \right] \right) = \left(\prod_{i=1}^{\ell} \frac{1}{1-k_i} \right) \text{sv}(f_{k_1-1} f_{k_2-1} \dots f_{k_\ell-1}) \text{ mod lower depth}, \quad (4.22)$$

for their highest-depth terms, where words of length $< \ell$ in the f -alphabet have been dropped. This is confirmed by (see (3.7) to (3.9))

$$\rho \left(c^{\text{sv}} \left[\begin{matrix} k-2 \\ k \end{matrix} \right] \right) = \frac{1}{1-k} \text{sv}(f_{k-1}), \quad \rho \left(c^{\text{sv}} \left[\begin{matrix} 2 & 2 \\ 4 & 4 \end{matrix} \right] \right) = \frac{1}{9} \text{sv}(f_3 f_3), \quad \rho \left(c^{\text{sv}} \left[\begin{matrix} 2 & 4 \\ 4 & 6 \end{matrix} \right] \right) = \frac{1}{15} \text{sv}(f_3 f_5) \quad (4.23)$$

as well as the irreducible depth-three MZVs in (3.10)

$$\begin{aligned}
 \rho(c^{\text{sv}}[\begin{smallmatrix} 2 & 2 & 4 \\ 4 & 4 & 6 \end{smallmatrix}]) &= -\frac{1}{45} \text{sv}(f_3 f_3 f_5) - \frac{14573}{43200} f_{11}, \\
 \rho(c^{\text{sv}}[\begin{smallmatrix} 2 & 4 & 4 \\ 4 & 6 & 6 \end{smallmatrix}]) &= -\frac{1}{75} \text{sv}(f_3 f_5 f_5) + \frac{35071931}{124380000} f_{13}, \\
 \rho(c^{\text{sv}}[\begin{smallmatrix} 2 & 2 & 6 \\ 4 & 4 & 8 \end{smallmatrix}])) &= -\frac{1}{63} \text{sv}(f_3 f_3 f_7) - \frac{365983}{2708720} f_{13}.
 \end{aligned}
 \tag{4.24}$$

This resonates with the results of Saad in Lemma 12.3 of [73], where motivic iterated Eisenstein integrals over $G_{k_1}(\tau_1)G_{k_2}(\tau_2)\dots G_{k_\ell}(\tau_\ell)$ are related to \mathbb{Q} -multiples of $f_{k_\ell-1}\dots f_{k_2-1}f_{k_1-1}$ upon translating MZVs into the f -alphabet and discarding lower-depth terms. These iterated Eisenstein integrals arise as multiple modular values in the S -cocycle of $\beta^{\text{sv}}[\begin{smallmatrix} j_1 & \dots & j_\ell \\ k_1 & \dots & k_\ell \end{smallmatrix}]$ and need to be cancelled by the corresponding c^{sv} in the modular completions β^{eqv} . The single-valued map of the f_i encountered in (4.22) can be traced back to the combination of holomorphic and antiholomorphic iterated Eisenstein integrals and the associated multiple modular values in the expression (2.14) for β^{sv} .

It would be interesting if all-order formulae similar to (4.24) could be found for c^{sv} with subleading entries $j_i < k_i - 2$ which still feature irreducible single-valued MZVs beyond depth one. The simplest depth-three examples of this type are $c^{\text{sv}}[\begin{smallmatrix} j_1 & j_2 & j_3 \\ 4 & 6 & 6 \end{smallmatrix}]$ at $j_1 + j_2 + j_3 = 8$ (rather than 10), where for instance

$$\begin{aligned}
 c^{\text{sv}}[\begin{smallmatrix} 0 & 4 & 4 \\ 4 & 6 & 6 \end{smallmatrix}] &= -\frac{\zeta_{3,5,3}^{\text{sv}}}{31500} + \frac{\zeta_3^2 \zeta_5}{1575} - \frac{31\zeta_{11}}{94500}, \\
 \rho(c^{\text{sv}}[\begin{smallmatrix} 0 & 4 & 4 \\ 4 & 6 & 6 \end{smallmatrix}])) &= \frac{1}{3150} \text{sv}(f_3 f_3 f_5 + f_3 f_5 f_3) - \frac{232}{23625} f_{11}.
 \end{aligned}
 \tag{4.25}$$

4.2 Comparison with the construction via β^{sv}

In order to compare the new generating function (4.2) of the modular forms β^{eqv} with their earlier construction in terms of β^{sv} , we also cast (3.3) and (2.14) into generating-function form,

$$J^{\text{eqv}}(\{\epsilon_k\}; \tau) = J_+(\{\epsilon_k\}; \tau) \widetilde{J}_-(\{\epsilon_k\}; \tau) \mathcal{K}(\{\epsilon_k\}; \tau) D^{\text{sv}}(\{\epsilon_k\}; \tau).
 \tag{4.26}$$

The cancellation of cusp-form contributions is again incorporated through the relations among the derivations ϵ_k . The combinations d^{sv} and $\bar{\kappa}$ of constants c^{sv} and antiholomorphic T -invariants $\bar{\alpha}$ in (3.4) and (2.16) are generated by

$$D^{\text{sv}}(\{\epsilon_k\}; \tau) = \sum_P \epsilon[P] d^{\text{sv}}[P; \tau], \quad \mathcal{K}(\{\epsilon_k\}; \tau) = \sum_P \epsilon[P] \overline{\kappa[P; \tau]}.
 \tag{4.27}$$

In fact, all of D^{sv} , \mathcal{K} and the product $J_+ \widetilde{J}_-$ in (4.26) are individually T invariant. This is different from (4.2), where the series B^{sv} of single-valued MZVs in (4.6) depends on both $\text{Re } \tau$ and $\text{Im } \tau$ with a non-trivial T -variation.

The goal of this section is to compare the two presentations (4.26) and (4.2) of the generating series of modular forms β^{eqv} . In particular, we will describe the antiholomorphic T -invariants $\overline{\alpha}[\dots; \tau]$ in the earlier construction of β^{sv} from the perspective of Brown's work by equating (4.26) with (4.2)

$$\widetilde{J}_-(\{\epsilon_k\}; \tau) \mathcal{K}(\{\epsilon_k\}; \tau) D^{\text{sv}}(\{\epsilon_k\}; \tau) = B^{\text{sv}}(\{\epsilon_k\}; \tau) \phi^{\text{sv}}(\widetilde{J}_-(\{\epsilon_k\}; \tau))
 \tag{4.28}$$

and solving for the generating series $\mathcal{K}(\{\epsilon_k\}; \tau)$ of the $\overline{\alpha[\dots; \tau]}$ in (2.16)

$$\mathcal{K}(\{\epsilon_k\}; \tau) = \widetilde{J}_-(\{\epsilon_k\}; \tau)^{-1} B^{\text{sv}}(\{\epsilon_k\}; \tau) \phi^{\text{sv}}(\widetilde{J}_-(\{\epsilon_k\}; \tau)) D^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1}. \quad (4.29)$$

The inversion of the series \widetilde{J}_- and D^{sv} can be readily implemented by reversing the entries P of their coefficients and inserting minus signs for the $|P|$ number of letters $\overset{j}{k}$ in P , i.e. by employing

$$\left(\sum_P \epsilon[P] C[P] \right)^{-1} = \sum_P (-1)^{|P|} \epsilon[P] C[P^t] \quad (4.30)$$

for arbitrary coefficients $C[P]$ subject to shuffle relations $C[X]C[Y] = \sum_{P \in X \sqcup Y} C[P]$. Hence, the components of (4.29) yield

$$\overline{\kappa[P; \tau]} = \sum_{P=WXYZ} (-1)^{|W|+|Z|} d^{\text{sv}}[W^t; \tau] \beta_-^\phi[X^t; \tau] b^{\text{sv}}[Y; \tau] \beta_-[Z; \tau], \quad (4.31)$$

which determine the antiholomorphic T -invariants $\overline{\alpha[\dots; \tau]}$ through the inverse

$$\overline{\alpha \left[\begin{array}{c} \dots j_i \dots \\ \dots k_i \dots \end{array}; \tau \right]} = \sum_{p_i=0}^{k_i-2-j_i} \frac{\binom{k_i-2-j_i}{p_i}}{(-4y)^{p_i}} \overline{\kappa \left[\begin{array}{c} \dots j_i+p_i \dots \\ \dots k_i \dots \end{array}; \tau \right]} \quad (4.32)$$

of the transformation (2.16) with one summation over p_i per column. The depth-one version of the deconcatenation formula (4.31) is not sensitive to the reversals of W and X , and one can easily verify the vanishing of

$$\overline{\kappa \left[\begin{array}{c} j \\ k \end{array} \right]} = \beta_-^\phi \left[\begin{array}{c} j \\ k \end{array} \right] - \beta_- \left[\begin{array}{c} j \\ k \end{array} \right] + b^{\text{sv}} \left[\begin{array}{c} j \\ k \end{array} \right] - d^{\text{sv}} \left[\begin{array}{c} j \\ k \end{array} \right] = 0 \quad (4.33)$$

since both $b^{\text{sv}} \left[\begin{array}{c} j \\ k \end{array} \right] - d^{\text{sv}} \left[\begin{array}{c} j \\ k \end{array} \right]$ and $\beta_-^\phi \left[\begin{array}{c} j \\ k \end{array} \right] - \beta_- \left[\begin{array}{c} j \\ k \end{array} \right]$ cancel in view of (3.7), (4.4) and (4.16). In the following, we shall express $\overline{\kappa[\dots; \tau]}$ at depths two and three in terms of the objects $d^{\text{sv}}, \beta_-^\phi, b^{\text{sv}}, \beta_-$ related to Brown's construction. Together with the all-order results for the $\overline{\alpha[\dots; \tau]}$ in (3.21) and appendix B, the subsequent depth-two and depth-three expressions were the central piece of evidence for the equivalence of the two constructions (3.3) and (4.14) of modular forms β^{eqv} .

4.2.1 Depth two

The expression (4.31) for $\overline{\kappa[P; \tau]}$ at depth $|P| = 2$ simplifies to

$$\begin{aligned} \overline{\kappa \left[\begin{array}{cc} j_1 & j_2 \\ k_1 & k_2 \end{array} \right]} &= \beta_- \left[\begin{array}{cc} j_1 & j_2 \\ k_1 & k_2 \end{array} \right] - \beta_- \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] \beta_-^\phi \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] + \beta_-^\phi \left[\begin{array}{cc} j_2 & j_1 \\ k_2 & k_1 \end{array} \right] + b^{\text{sv}} \left[\begin{array}{cc} j_1 & j_2 \\ k_1 & k_2 \end{array} \right] - b^{\text{sv}} \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] d^{\text{sv}} \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] + d^{\text{sv}} \left[\begin{array}{cc} j_2 & j_1 \\ k_2 & k_1 \end{array} \right] \\ &\quad + \beta_-^\phi \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] b^{\text{sv}} \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] - b^{\text{sv}} \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] \beta_- \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] + d^{\text{sv}} \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] \left(\beta_- \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] - \beta_-^\phi \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] \right) \\ &= \delta_\phi \beta_- \left[\begin{array}{cc} j_2 & j_1 \\ k_2 & k_1 \end{array} \right] + \beta_- \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] d^{\text{sv}} \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] - d^{\text{sv}} \left[\begin{array}{c} j_1 \\ k_1 \end{array} \right] \beta_- \left[\begin{array}{c} j_2 \\ k_2 \end{array} \right] + b^{\text{sv}} \left[\begin{array}{cc} j_1 & j_2 \\ k_1 & k_2 \end{array} \right] - d^{\text{sv}} \left[\begin{array}{cc} j_1 & j_2 \\ k_1 & k_2 \end{array} \right], \end{aligned} \quad (4.34)$$

with $d^{\text{sv}} \left[\begin{array}{c} j \\ k \end{array} \right]$ given by (3.7). In passing to the last line, we have used the agreement of β_-^ϕ, β_- and $b^{\text{sv}}, d^{\text{sv}}$ at depth one as well as the shuffle property of β_- and d^{sv} .

The various terms in (4.34) have different interpretations and combine in such a way as to make this expression T -invariant even though this invariance is not manifest term by

term. More precisely, the first three terms involving $\delta_\phi\beta_-$ and β_- yield antiholomorphic iterated Eisenstein integrals at depth one with odd zeta values in their coefficients due to ϕ^{sv} or the accompanying d^{sv} . The difference $b^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right] - d^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right]$ at the end of (4.34) has depth zero from the viewpoint of Eisenstein integrals and introduces ratios $\bar{\tau}^\ell/y^p$ as in (4.3) with at least one power $\ell \geq 1$ of $\bar{\tau}$. The relative factors and MZV coefficients of depth-one and depth-zero contributions play out to recombine every term into the T -invariant integrals $\overline{\mathcal{E}_0(\dots; \tau)}$ in (3.19), multiplied by non-positive powers of y .

When extracting $\overline{\alpha\left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right]}$ from (4.34) via (4.32), we can clearly identify the sources of the two contributions $\overline{\alpha_{\text{easy}}}$ and $\overline{\alpha_{\text{hard}}}$ in the all-order formula (3.21):

- The simple expression for $\overline{\alpha_{\text{easy}}}$ in (3.21) can be traced back to the second and third term $\beta_- \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}\right] - d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] \beta_- \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}\right]$ in the last line of (4.34).
- The generating function (3.22) of $\overline{\alpha_{\text{hard}}}$ stems from the $\delta_\phi\beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right]$ in (4.34) which are already fixed by the contributions $\sim \zeta_{i_1}[z_{i_1}, \epsilon_k]$ to $\phi^{\text{sv}}(\epsilon_k)$ in (4.11) and obey the closed formula (4.20).

In both cases, the depth-zero terms $b^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right] - d^{\text{sv}}\left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right]$ in (4.34) ensure that the antiholomorphic Eisenstein integrals in $\beta_- \left[\begin{smallmatrix} j \\ k \end{smallmatrix}\right]$ and $\delta_\phi\beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right]$ conspire to reconstruct $\overline{\mathcal{E}_0}$.

Conversely, the generating function (3.22) of $\overline{\alpha_{\text{hard}}}$ inferred from inspecting the variety of examples in [43] was crucial in the early stages of this work to anticipate the significance of the derivations z_3, z_5, \dots in the closed-form expression (4.12) for ϕ^{sv} . While the matching of $\overline{\alpha_{\text{hard}}}$ with $\delta_\phi\beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right]$ guided the identification of $\zeta_{i_1}[z_{i_1}, \epsilon_k]$ -contributions to $\phi^{\text{sv}}(\epsilon_k)$, the second order $\zeta_{i_1}\zeta_{i_2}[z_{i_1}, [z_{i_2}, \epsilon_k]]$ firstly became accessible from the depth-three analysis in the next section.

4.2.2 Depth three

By suitably assembling the $\overline{\kappa[P; \tau]}$ at depth $|P| = 3$ from (4.31), we have

$$\begin{aligned}
 \overline{\kappa\left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}\right]} &= \beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] + \beta_- \left[\begin{smallmatrix} j_2 & j_3 \\ k_2 & k_3 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] - \beta_- \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] \beta_- \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}\right] \\
 &\quad - \beta_- \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] + \left(d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}\right] - b^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}\right] \right) \beta_- \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] \\
 &\quad + \beta_- \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] b^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_3 \\ k_2 & k_3 \end{smallmatrix}\right] + \delta_\phi\beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] - d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] \delta_\phi\beta_- \left[\begin{smallmatrix} j_3 & j_2 \\ k_3 & k_2 \end{smallmatrix}\right] \quad (4.35) \\
 &\quad + \delta_\phi\beta_- \left[\begin{smallmatrix} j_3 & j_2 & j_1 \\ k_3 & k_2 & k_1 \end{smallmatrix}\right] \Big|_{\text{depth } 1} + \delta_\phi\beta_- \left[\begin{smallmatrix} j_3 & j_2 & j_1 \\ k_3 & k_2 & k_1 \end{smallmatrix}\right] \Big|_{\text{depth } 2} - \delta_\phi\beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right] \beta_- \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] \\
 &\quad + b^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}\right] - d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}\right] b^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_3 \\ k_2 & k_3 \end{smallmatrix}\right] + d^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right] d^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right] - d^{\text{sv}} \left[\begin{smallmatrix} j_3 & j_2 & j_1 \\ k_3 & k_2 & k_1 \end{smallmatrix}\right].
 \end{aligned}$$

As will be explained in appendix B, the detailed structure of (4.35) harmonizes with an all-weight formula for $\overline{\alpha[\dots; \tau]}$ of depth three. The right-hand side features β_- of depth $0 \leq \ell \leq 2$, for instance, depth-two integrals in the first line and in the contributions $\delta_\phi\beta_- \left[\begin{smallmatrix} j_3 & j_2 & j_1 \\ k_3 & k_2 & k_1 \end{smallmatrix}\right] \Big|_{\text{depth } 2} - \delta_\phi\beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix}\right] \beta_- \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}\right]$ to the fourth line. The last line of (4.35) in turn has depth zero and again features at least one power of $\bar{\tau}$ in each term.

4.2.3 Comparison with Brown’s single-valued iterated Eisenstein integrals

According to section 8.1 of [37], right-multiplication of the series J^{eqv} of EIEIs with $(B^{\text{sv}})^{-1}$ yields Brown’s *single-valued iterated Eisenstein integrals*,

$$\begin{aligned} J^{\text{sv}}(\{\epsilon_k\}; \tau) &= J^{\text{eqv}}(\{\epsilon_k\}; \tau) B^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1} \\ &= J_+(\{\epsilon_k\}; \tau) B^{\text{sv}}(\{\epsilon_k\}; \tau) \phi^{\text{sv}}(\widetilde{J}_-(\{\epsilon_k\}; \tau)) B^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1}, \end{aligned} \tag{4.36}$$

that, using (4.13), can also be written as

$$J^{\text{sv}}(\{\epsilon_k\}; \tau) = J_+(\{\epsilon_k\}; \tau) \mathbb{N}^{\text{sv}} \widetilde{J}_-(\{\epsilon_k\}; \tau) (\mathbb{N}^{\text{sv}})^{-1}, \tag{4.37}$$

where $\mathbb{N}^{\text{sv}} = B^{\text{sv}}(\{\epsilon_k\}; \tau) \mathbb{M}^{\text{sv}}$ depends on both the ϵ_k and z_m . The freedom to redefine $B^{\text{sv}} \rightarrow B^{\text{sv}} a^{-1}$ and $\phi^{\text{sv}}(\widetilde{J}_-) \rightarrow a \phi^{\text{sv}}(\widetilde{J}_-) a^{-1}$ discussed below (4.13) amounts to the left-multiplication $\mathbb{M}^{\text{sv}} \rightarrow a \mathbb{M}^{\text{sv}}$ and therefore drops out from the product $\mathbb{N}^{\text{sv}} = B^{\text{sv}} \mathbb{M}^{\text{sv}}$. That is why J^{sv} is canonically defined and does admit redefinitions analogous to $J^{\text{eqv}} \rightarrow J^{\text{eqv}} a^{-1}$ [37].

The form (4.37) is reminiscent of known constructions of single-valued functions and periods (e.g. [38, 64, 74, 75]), which are made up of a combination of holomorphic and anti-holomorphic parts where the anti-holomorphic parts are transformed using for example — in the case of generating functions — a conjugation.

The expansion of J^{sv} is to be contrasted with the generating series of the β^{sv} in the physics literature

$$\begin{aligned} \sum_P \beta^{\text{sv}}[P; \tau] \epsilon[P] &= J^{\text{eqv}}(\{\epsilon_k\}; \tau) D^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1} \\ &= J_+(\{\epsilon_k\}; \tau) B^{\text{sv}}(\{\epsilon_k\}; \tau) \phi^{\text{sv}}(\widetilde{J}_-(\{\epsilon_k\}; \tau)) D^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1}, \end{aligned} \tag{4.38}$$

which follows from (2.14) and (4.28) and features a right-multiplicative inverse $D^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1}$ instead of the $B^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1}$ in (4.36). Thus it follows that

$$J^{\text{sv}}(\{\epsilon_k\}; \tau) = \left(\sum_P \beta^{\text{sv}}[P; \tau] \epsilon[P] \right) D^{\text{sv}}(\{\epsilon_k\}; \tau) B^{\text{sv}}(\{\epsilon_k\}; \tau)^{-1}. \tag{4.39}$$

The depth-one components $b^{\text{sv}} \begin{bmatrix} j \\ k \end{bmatrix} = d^{\text{sv}} \begin{bmatrix} j \\ k \end{bmatrix}$ still happen to agree, and $\beta^{\text{sv}} \begin{bmatrix} j \\ k \end{bmatrix}$ coincide with Brown’s single-valued iterated Eisenstein integrals at depth one. At depth $\ell \geq 2$, however, the b^{sv} generically depart from d^{sv} by the polynomial dependence on $\bar{\tau}$ in (4.3). Hence, by the mismatch between (4.36) and (4.38), the $\beta^{\text{sv}} \begin{bmatrix} j_1 \dots j_\ell \\ k_1 \dots k_\ell \end{bmatrix}$ at $\ell \geq 2$ differ from Brown’s single-valued iterated Eisenstein integrals by terms involving at least one non-trivial MZV and one power of $\bar{\tau}$ in the numerator. One may view the β^{sv} as T -invariantized versions of Brown’s single-valued iterated Eisenstein integrals since, in contrast to the inverse B^{sv} in (4.36), the series D^{sv} in (4.38) is invariant under $\tau \rightarrow \tau+1$.

4.3 Relation to Brown’s equivariant double iterated integrals

So far, we have only matched the subspace of the modular forms β^{eqv} with Brown’s work, where iterated integrals involving holomorphic cusp forms are projected out by the

accompanying ϵ_k . In this section, we go beyond this subspace and connect the cusp-form contributions $\beta_{\Delta}^{\text{sv}}$ to β^{eqv} of depth two in (3.2) and (3.28) with Brown's equivariant double iterated integrals of [36].

Following the normalization conventions in the reference, Brown's double integrals are constructed from holomorphic $(1, 0)$ -forms⁸

$$\underline{\mathbf{G}}_k[X, Y; \tau] = \frac{(k-1)!}{2(2\pi i)^{k-1}} (X - \tau Y)^{k-2} \mathbf{G}_k(\tau) d\tau \tag{4.40}$$

involving commutative bookkeeping variables X, Y . These one-forms are in fact, multiples of the generating functions (2.13) of the earlier forms $\omega_{\pm} \left[\begin{smallmatrix} j \\ k \end{smallmatrix}; \tau, \tau_1 \right]$ in (2.10). Accordingly, iterated integrals of $\underline{\mathbf{G}}_{k_1}[X_1, Y_1; \tau_1] \underline{\mathbf{G}}_{k_2}[X_2, Y_2; \tau_2] \dots$ generate the constituents β_{\pm} of MGFs in (2.15) upon expansion in the combinations $(X_i - \tau Y_i)^{j_i} (X_i - \bar{\tau} Y_i)^{k_i - j_i - 2}$ [36].

At depth one, the real-analytic combinations

$$M_k[X, Y; \tau] = -\frac{1}{2} \int_{\tau}^{i\infty} \underline{\mathbf{G}}_k[X, Y; \tau_1] - \frac{1}{2} \int_{\bar{\tau}}^{-i\infty} \overline{\underline{\mathbf{G}}_k[X, Y; \tau_1]} + \frac{(k-2)! \zeta_{k-1}}{2(2\pi i)^{k-2}} Y^{k-2} \tag{4.41}$$

with $k \geq 4$ as well as $\bar{X} = X$ and $\bar{Y} = Y$ generate non-holomorphic Eisenstein series (3.14) via

$$M_k[X, Y; \tau] = -\frac{1}{4} (k-1)! \sum_{j=0}^{k-2} \frac{\binom{k-2}{j}}{(-4y)^j} \beta^{\text{eqv}} \left[\begin{smallmatrix} j \\ k \end{smallmatrix}; \tau \right] (X - \tau Y)^j (X - \bar{\tau} Y)^{k-2-j}, \tag{4.42}$$

where the additive constant $\sim Y^{k-2}$ in (4.41) (not to be confused with $y = \pi \text{Im } \tau$) introduces the odd zeta value into the modular forms β^{eqv} of depth one in (3.1) [36]. The object (4.42) is referred to as an equivariant Eisenstein integral since the action on the bookkeeping variables (X, Y) leads to the $\text{SL}(2, \mathbb{Z})$ invariance

$$M_k \left[aX + bY, cX + dY; \frac{a\tau + b}{c\tau + d} \right] = M_k[X, Y; \tau]. \tag{4.43}$$

4.3.1 The non-modular primitives at depth two

At depth two, Brown's construction [36] of equivariant double iterated integrals starts from closed one-forms $\sim \underline{\mathbf{G}}_{k_1}[X_1, Y_1; \tau] M_{k_2}[X_2, Y_2; \tau] + M_{k_1}[X_1, Y_1; \tau] \overline{\underline{\mathbf{G}}_{k_2}[X_2, Y_2; \tau]}$ and considers their real-analytic primitive

$$\begin{aligned} K_{k_1, k_2}[X_1, Y_1, X_2, Y_2; \tau] = & \tag{4.44} \\ & \frac{1}{4} \int_{\tau}^{i\infty} \underline{\mathbf{G}}_{k_1}[X_1, Y_1; \tau_1] \int_{\tau_1}^{i\infty} \underline{\mathbf{G}}_{k_2}[X_2, Y_2; \tau_2] \\ & + \frac{1}{4} \int_{\tau}^{i\infty} \underline{\mathbf{G}}_{k_1}[X_1, Y_1; \tau_1] \int_{\bar{\tau}}^{-i\infty} \overline{\underline{\mathbf{G}}_{k_2}[X_2, Y_2; \tau_2]} + \frac{1}{4} \int_{\bar{\tau}}^{-i\infty} \overline{\underline{\mathbf{G}}_{k_2}[X_2, Y_2; \tau_2]} \int_{\bar{\tau}_2}^{-i\infty} \overline{\underline{\mathbf{G}}_{k_1}[X_1, Y_1; \tau_1]} \\ & - \frac{(k_2-2)! \zeta_{k_2-1}}{4(2\pi i)^{k_2-2}} Y_2^{k_2-2} \int_{\tau}^{i\infty} \underline{\mathbf{G}}_{k_1}[X_1, Y_1; \tau_1] - \frac{(k_1-2)! \zeta_{k_1-1}}{4(2\pi i)^{k_1-2}} Y_1^{k_1-2} \int_{\bar{\tau}}^{-i\infty} \overline{\underline{\mathbf{G}}_{k_2}[X_2, Y_2; \tau_2]}, \end{aligned}$$

⁸The expressions (4.40) for $\underline{\mathbf{G}}_k[X, Y; \tau]$ and (4.41) below for $M_k[X, Y; \tau]$ are denoted by \underline{E}_k and \mathcal{E}_{k-2} in [36].

where we have rewritten the integrals of the reference in a manifestly homotopy-invariant way. In order to avoid cluttering, we shall no longer spell out the dependence of K_{k_1, k_2} and related objects on the commutative bookkeeping variables X_i, Y_i . By decomposing the integration kernels $X_i - \tau_i Y_i$ and $X_i - \bar{\tau}_i Y_i$ as in (2.13), one can rewrite (4.44) as

$$\begin{aligned}
 K_{k_1, k_2} = & \frac{(k_1-1)!(k_2-1)!}{16} \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \frac{\binom{k_1-2}{j_1} \binom{k_2-2}{j_2}}{(-4y)^{j_1+j_2}} \left(\beta_+ \begin{bmatrix} j_2 & j_1 \\ k_2 & k_1 \end{bmatrix} - \beta_+ \begin{bmatrix} j_1 \\ k_1 \end{bmatrix} \beta_- \begin{bmatrix} j_2 \\ k_2 \end{bmatrix} + \beta_- \begin{bmatrix} j_1 & j_2 \\ k_1 & k_2 \end{bmatrix} \right) \\
 & \times (X_1 - \tau Y_1)^{j_1} (X_1 - \bar{\tau} Y_1)^{k_1-2-j_1} (X_2 - \tau Y_2)^{j_2} (X_2 - \bar{\tau} Y_2)^{k_2-2-j_2} \tag{4.45} \\
 & - \frac{(k_2-2)!(k_1-1)! \zeta_{k_2-1}}{8(2\pi i)^{k_2-2}} \sum_{j=0}^{k_1-2} \binom{k_1-2}{j} \frac{(-1)^j}{(4y)^j} \beta_+ \begin{bmatrix} j \\ k_1 \end{bmatrix} (X_1 - \tau Y_1)^j (X_1 - \bar{\tau} Y_1)^{k_1-2-j} Y_2^{k_2-2} \\
 & - \frac{(k_1-2)!(k_2-1)! \zeta_{k_1-1}}{8(2\pi i)^{k_1-2}} \sum_{j=0}^{k_2-2} \binom{k_2-2}{j} \frac{(-1)^j}{(4y)^j} \beta_- \begin{bmatrix} j \\ k_2 \end{bmatrix} Y_1^{k_1-2} (X_2 - \tau Y_2)^j (X_2 - \bar{\tau} Y_2)^{k_2-2-j},
 \end{aligned}$$

where the round bracket in the first line features $\beta^{\text{sv}} \begin{bmatrix} j_2 & j_1 \\ k_2 & k_1 \end{bmatrix}$ up to the lower-depth contributions from $\overline{\alpha[\dots; \tau]}$ in (2.12). One can anticipate from the variety of lower-depth terms in the constructions (3.2) or (4.21) of modular forms $\beta^{\text{eqv}} \begin{bmatrix} j_1 & j_2 \\ k_1 & k_2 \end{bmatrix}$ that (4.45) is not yet equivariant in the sense of (4.43).

4.3.2 The modular completion at depth two

In the same way as the additive constant $\zeta_{k-1} Y^{k-2}$ in (4.41) ensures equivariance of M_k at depth one, there is a systematic modular completion M_{k_1, k_2} of K_{k_1, k_2} in (4.44) and (4.45): on top of a polynomial c_{k_1, k_2}^γ in X_i, Y_i independent on τ , the additional complexity at depth two generically requires the addition of holomorphic and antiholomorphic depth-one integrals [36],

$$M_{k_1, k_2} = K_{k_1, k_2} - c_{k_1, k_2}^\gamma - \frac{1}{2} \left\{ \int_\tau^{i\infty} \underline{f}_{k_1, k_2}^0(\tau_1) + \int_{\bar{\tau}}^{-i\infty} \overline{\underline{g}_{k_1, k_2}^0(\tau_1)} + \int_{\bar{\tau}}^{-i\infty} \overline{\underline{g}_{k_1, k_2}^{\text{E}}(\tau_1)} \right\}. \tag{4.46}$$

As detailed in the reference, $\underline{f}_{k_1, k_2}^0(\tau_1)$ is an equivariant $(1, 0)$ -form in τ_1 while $\overline{\underline{g}_{k_1, k_2}^0(\tau_1)}$ and $\overline{\underline{g}_{k_1, k_2}^{\text{E}}(\tau_1)}$ are equivariant $(0, 1)$ -forms in τ_1 composed of⁹

- a holomorphic cusp form $\Delta_{2s}(\tau_1)$ in the case of $\underline{f}_{k_1, k_2}^0(\tau_1)$
- an antiholomorphic cusp form $\overline{\Delta_{2s}(\tau_1)}$ in the case of $\overline{\underline{g}_{k_1, k_2}^0(\tau_1)}$ and an antiholomorphic Eisenstein series $\overline{G_k(\tau_1)}$ in the case of $\overline{\underline{g}_{k_1, k_2}^{\text{E}}(\tau_1)}$
- a polynomial in the bookkeeping variables X_i, Y_i as well as τ_1 in the case of $\underline{f}_{k_1, k_2}^0(\tau_1)$ or $\bar{\tau}_1$ in the case of $\overline{\underline{g}_{k_1, k_2}^0(\tau_1)}$ or $\overline{\underline{g}_{k_1, k_2}^{\text{E}}(\tau_1)}$

All of c_{k_1, k_2}^γ , $\underline{f}_{k_1, k_2}^0(\tau_1)$, $\overline{\underline{g}_{k_1, k_2}^0(\tau_1)}$ and $\overline{\underline{g}_{k_1, k_2}^{\text{E}}(\tau_1)}$ are understood to have homogeneity degrees k_1-2 in X_1, Y_1 and k_2-2 in X_2, Y_2 compatible with K_{k_1, k_2} in (4.44). As detailed in section 9.2

⁹In [36], the antiholomorphic forms $\overline{\underline{g}_{k_1, k_2}^0(\tau_1)}$ and $\overline{\underline{g}_{k_1, k_2}^{\text{E}}(\tau_1)}$ are combined into a single object, but we find it useful to separate their contributions. We have also introduced a superscript ⁰ for the cuspidal parts compared to the notation in [36].

of [36], the existence of modular completions M_{k_1, k_2} in (4.46) for any $k_1, k_2 \in 2\mathbb{N}+2$ follows from the Eichler-Shimura theorem [76, 77]. At depth one, in turn, the contribution $\zeta_{k-1} Y^{k-2}$ to (4.41) already suffices to compensate the $\text{SL}(2, \mathbb{Z})$ -transformation (or ‘‘cocycle’’) of the $\overline{\mathbf{G}_k[\dots]}$ - and $\overline{\mathbf{G}_k[\dots]}$ integrals: the cocycle of the real-analytic combination of Eisenstein integrals in (4.41) is a coboundary [35].

The modular completion $K_{k_1, k_2} \rightarrow M_{k_1, k_2}$ in (4.46) assembles exactly the kinds of constituents needed to convert the β_{\pm} in (4.45) to the modular forms $\beta^{\text{eqv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$:

- The $\mathbb{Q}[(2\pi i)^{-1}]$ -linear combinations of MZVs in the coefficients of c_{k_1, k_2}^{γ} generate the depth-zero terms $b^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$ in (4.21).
- The Eisenstein part $\overline{\mathbf{g}_{k_1, k_2}^{\text{E}}}(\tau_1)$ yields the contribution $\delta_{\phi} \beta_{-} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix} \right]$ to (4.21) from the change of alphabet ϕ^{sv} in section 4.1.2. We therefore find non-zero $\overline{\mathbf{g}_{k_1, k_2}^{\text{E}}}(\tau_1)$ for any pair $k_1, k_2 \in 2\mathbb{N}+2$ subject to $k_1 \neq k_2$.
- Finally, $\mathbf{f}_{k_1, k_2}^0(\tau_1)$ and $\overline{\mathbf{g}_{k_1, k_2}^0}(\tau_1)$ combine to the contributions $\beta_{\Delta}^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix} \right]$ to (4.21) and vanish for $k_1 + k_2 < 14$. More precisely, the holomorphic and antiholomorphic integrals in (3.30) are captured by $\mathbf{f}_{k_1, k_2}^0(\tau_1)$ and $\overline{\mathbf{g}_{k_1, k_2}^0}(\tau_1)$, respectively.

On these grounds, it is not surprising that the transition from K_{k_1, k_2} to M_{k_1, k_2} promotes the depth-two terms in the first line of (4.45) to $\beta^{\text{eqv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$,

$$M_{k_1, k_2} = \frac{1}{16} (k_1 - 1)! (k_2 - 1)! \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \frac{\binom{k_1-2}{j_1} \binom{k_2-2}{j_2}}{(-4y)^{j_1+j_2}} \beta^{\text{eqv}} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix} \right] \quad (4.47)$$

$$\times (X_1 - \tau Y_1)^{j_1} (X_1 - \bar{\tau} Y_1)^{k_1-2-j_1} (X_2 - \tau Y_2)^{j_2} (X_2 - \bar{\tau} Y_2)^{k_2-2-j_2} .$$

Moreover, since the relation between b^{sv} and c^{sv} in (4.3) implements the change of alphabet between $(X_i - \tau Y_i), (X_i - \bar{\tau} Y_i)$ and X_i, Y_i , we can express the constant c_{k_1, k_2}^{γ} in (4.46) as

$$c_{k_1, k_2}^{\gamma} = -\frac{1}{16} (k_1 - 1)! (k_2 - 1)! \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \binom{k_1-2}{j_1} \binom{k_2-2}{j_2} c^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix} \right]$$

$$\times \left(\frac{iY_1}{2\pi} \right)^{j_1} X_1^{k_1-2-j_1} \left(\frac{iY_2}{2\pi} \right)^{j_2} X_2^{k_2-2-j_2} . \quad (4.48)$$

Finally, the Eisenstein part $\overline{\mathbf{g}_{k_1, k_2}^{\text{E}}}(\tau)$ can be given in the closed form

$$\overline{\mathbf{g}_{k_1, k_2}^{\text{E}}}(\tau) = \begin{cases} -\frac{\zeta_{k_1-1} (k_1-2)! (k_2-k_1+1) (k_2-k_1+2) \mathbf{B}_{k_2}}{2(2\pi i)^{k_1-2} k_2 (k_2-1) \mathbf{B}_{k_2-k_1+2}} \\ \quad \times (X_1 Y_2 - X_2 Y_1)^{k_1-2} \overline{\mathbf{G}_{k_2-k_1+2}}[X_2, Y_2; \tau] : k_1 < k_2, \\ \frac{\zeta_{k_2-1} (k_2-2)! (k_1-k_2+1) (k_1-k_2+2) \mathbf{B}_{k_1}}{2(2\pi i)^{k_2-2} k_1 (k_1-1) \mathbf{B}_{k_1-k_2+2}} \\ \quad \times (X_1 Y_2 - X_2 Y_1)^{k_2-2} \overline{\mathbf{G}_{k_1-k_2+2}}[X_1, Y_1; \tau] : k_2 < k_1, \\ 0 & : k_1 = k_2, \end{cases} , \quad (4.49)$$

see (4.40) for the definition of $\underline{G}_k[X, Y; \tau]$. As can be anticipated from the powers of the modular invariant $X_1Y_2 - X_2Y_1$, the Eisenstein integrals $\overline{\underline{G}_{k_2-k_1+2}[\dots]}$ only contribute to a single $SL(2, \mathbb{R})$ multiplet of MGFs that can be extracted from M_{k_1, k_2} through the projectors δ^k in section 7 of [36]. The $SL(2, \mathbb{R})$ representation theory of MGFs of depths two and three will be discussed in [45]. We have checked (4.47), (4.48) and (4.49) for all depth-two cases up to and including $k_1+k_2 = 28$.

4.3.3 On uniqueness of M_{k_1, k_2} and choices in J^{eqv}

As noted in section 9.2 of [36], the $SL(2, \mathbb{R})$ -singlet component of M_{k_1, k_2} may be shifted by a constant $c \in \mathbb{C}$ without altering the modular properties. Such singlets only occur in the case of $k_1=k_2=k$ and are then proportional to $(X_1Y_2 - X_2Y_1)^{k-2}$. Since k is even, the singlet will be symmetric under exchange of $X_1, Y_1 \leftrightarrow X_2, Y_2$ and therefore involve combinations $\beta^{\text{eqv}} \begin{bmatrix} j_1 & j_2 \\ k & k \end{bmatrix} + \beta^{\text{eqv}} \begin{bmatrix} j_2 & j_1 \\ k & k \end{bmatrix}$ in (4.47). These combinations conspire to the shuffles $\beta^{\text{eqv}} \begin{bmatrix} j_1 \\ k \end{bmatrix} \beta^{\text{eqv}} \begin{bmatrix} j_2 \\ k \end{bmatrix}$ which would no longer be the case when adding $c(X_1Y_2 - X_2Y_1)^{k-2}$ to $M_{k, k}$ and thereby redefining $\beta^{\text{eqv}} \begin{bmatrix} j_1 & j_2 \\ k & k \end{bmatrix} + \beta^{\text{eqv}} \begin{bmatrix} j_2 & j_1 \\ k & k \end{bmatrix}$. Hence, the ambiguity of adding a constant to the $SL(2, \mathbb{R})$ -singlet components at depth two is fixed by imposing shuffle relations between the components β^{eqv} of M_k and $M_{k, k}$.

Using this imposition, the modular completion given by equation (4.46) now uniquely determines the $c_{k_1, k_2}^\gamma, f_{k_1, k_2}^0(\tau_1), \overline{g_{k_1, k_2}^0(\tau_1)}$ and $\overline{g_{k_1, k_2}^E(\tau_1)}$. We note, however, that in this equation we have chosen the Eisenstein addition to appear in the form of $\overline{g_{k_1, k_2}^E(\tau_1)}$. We can, in fact, modify M_{k_1, k_2} by a suitable multiple of M_k to remove $\overline{g_{k_1, k_2}^E(\tau_1)}$ whilst retaining modular completion, but this will cause a function $f_{k_1, k_2}^E(\tau_1)$ composed of a holomorphic Eisenstein series to appear instead. The equation defining c_{k_1, k_2}^γ would also be affected by this modification.

The uniqueness argument for M_{k_1, k_2} also explains why the redefinitions $B^{\text{sv}} \rightarrow B^{\text{sv}} a^{-1}$ and $\phi^{\text{sv}}(\widetilde{J}_-) \rightarrow a \phi^{\text{sv}}(\widetilde{J}_-) a^{-1}$ by some series a in $\epsilon_k^{(j)}$ (with MZV coefficients) mentioned below (4.13) can be ruled out below depth three: only an $SL(2, \mathbb{R})$ singlet of modular forms β^{eqv} admits a redefinition of modular invariants by a constant from the series a without spoiling the differential equations (3.5) or (3.36). The absence of singlets at depth one rules out any components with a single factor of $\epsilon_k^{(j)}$ in a . Since the series a is imposed to be group like [37] (one would otherwise give up shuffle properties), the only viable depth-two contributions are commutators $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$. However, the latter do not contribute to the $SL(2, \mathbb{R})$ -singlet combination of β^{eqv} entering $M_{k, k}$ with $(X_1Y_2 - Y_1X_2)^{k-2}$ which rules out depth-two components in a .

At depth three, in turn, generic (k_1, k_2, k_3) admit $SL(2, \mathbb{R})$ -singlet combinations of modular forms $\beta^{\text{eqv}} \begin{bmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{bmatrix}$ that are independent under shuffle relations. That is why contributions $[\epsilon_{k_1}^{(j_1)}, [\epsilon_{k_2}^{(j_2)}, \epsilon_{k_3}^{(j_3)}]]$ to a compatible with the shuffle properties of β^{eqv} are conceivable such as the examples $\zeta_7[\epsilon_4^{(j_1)}, [\epsilon_4^{(j_2)}, \epsilon_6^{(j_3)}]]$ and $\zeta_3\zeta_5[\epsilon_6^{(j'_1)}, [\epsilon_6^{(j'_2)}, \epsilon_4^{(j'_3)}]]$ in the discussion below (4.13). This freedom of modifying depth-three contributions to J^{eqv} translates into depth-four modifications $\phi^{\text{sv}}(\widetilde{J}_-) \rightarrow a \phi^{\text{sv}}(\widetilde{J}_-) a^{-1}$ and can be fixed by imposing the change of alphabet ϕ^{sv} to take the form (4.12). Since we have not yet constructed the relevant β^{eqv} at depth four, we can only determine the preferred $c^{\text{sv}} \begin{bmatrix} j_1 & j_2 & j_3 \\ 4 & 4 & 6 \end{bmatrix}$ and $c^{\text{sv}} \begin{bmatrix} j_1 & j_2 & j_3 \\ 4 & 6 & 6 \end{bmatrix}$ up to one free

parameter each (see the supplementary material and the undetermined $c_{446} \in \mathbb{Q}$ in (3.18)) and relegate their fixing via (4.12) to the future. We stress that these free parameters merely concern canonical choices in shifting modular invariants by constants and do not reflect any shortcomings in the construction of modular forms at depth three or beyond.

4.3.4 Examples

The general discussion of Brown's equivariant double iterated integrals M_{k_1, k_2} calls for examples of the building blocks c_{k_1, k_2}^γ , $\mathfrak{f}_{k_1, k_2}^0(\tau)$, $\mathfrak{g}_{k_1, k_2}^0(\tau)$ and $\mathfrak{g}_{k_1, k_2}^E(\tau)$ of the modular completion in (4.46).

Based on the examples of single-valued MZVs $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$ of weight $(j_1 + j_2 + 2)$ in (3.8) and (3.9), the constants in (4.48) specialize to

$$\begin{aligned} c_{4,4}^\gamma &= -\frac{i\zeta_3}{960\pi} X_1 X_2 (X_1 Y_2 - X_2 Y_1) - \frac{5i\zeta_5}{192\pi^3} Y_1 Y_2 (X_1 Y_2 - X_2 Y_1) - \frac{\zeta_3^2}{32\pi^4} Y_1^2 Y_2^2, \\ c_{6,4}^\gamma &= \frac{i\zeta_3}{10080\pi} X_1^3 X_2 (2X_1 Y_2 - X_2 Y_1) - \frac{i\zeta_5}{960\pi^3} X_1 Y_1 (3X_2^2 Y_1^2 - 3X_1 X_2 Y_1 Y_2 + X_1^2 Y_2^2) \\ &\quad + \frac{\zeta_3^2}{112\pi^4} Y_1^2 (X_1 Y_2 - X_2 Y_1)^2 + \frac{7i\zeta_7}{128\pi^5} Y_1^3 Y_2 (X_1 Y_2 - X_2 Y_1) + \frac{3\zeta_3 \zeta_5}{32\pi^6} Y_1^4 Y_2^2 \end{aligned} \quad (4.50)$$

in case of double integrals over $G_4 G_4$ and $G_4 G_6$. Examples at higher weights can be generated from the list of all $c^{\text{sv}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix} \right]$ at $k_1 + k_2 \leq 28$ given in the supplementary material attached to this paper. We reiterate that the c^{sv} at depth two only involve odd zeta values and bilinears thereof, whereas irreducible single-valued MZVs beyond depth one are relegated to the modular completion of triple Eisenstein integrals and higher depth [73], see section 4.1.4.

The closed formula (4.49) for the Eisenstein part $\overline{\mathfrak{g}_{k_1, k_2}^E(\tau)}$ specializes as follows in the simplest non-vanishing examples

$$\begin{aligned} \overline{\mathfrak{g}_{4,6}^E(\tau)} &= -\frac{\zeta_3}{14\pi^2} (X_1 Y_2 - X_2 Y_1)^2 \overline{\mathbb{G}_4[X_2, Y_2; \tau]}, \\ \overline{\mathfrak{g}_{4,8}^E(\tau)} &= -\frac{3\zeta_3}{16\pi^2} (X_1 Y_2 - X_2 Y_1)^2 \overline{\mathbb{G}_6[X_2, Y_2; \tau]}, \\ \overline{\mathfrak{g}_{6,8}^E(\tau)} &= -\frac{9\zeta_5}{56\pi^4} (X_1 Y_2 - X_2 Y_1)^4 \overline{\mathbb{G}_4[X_2, Y_2; \tau]}. \end{aligned} \quad (4.51)$$

Finally, the cusp-form contributions $\mathfrak{f}_{k_1, k_2}^0(\tau)$, $\overline{\mathfrak{g}_{k_1, k_2}^0(\tau)}$ to (4.46) always arise in pairs by the structure of the $\beta^{\text{sv}} \left[\begin{smallmatrix} j \\ \Delta_k^\pm \end{smallmatrix}; \tau \right]$ in (3.28), (3.30) and are most conveniently expressed in terms of

$$\Delta_k \left[\begin{smallmatrix} X_1 & X_2 \\ Y_1 & Y_2 \\ r_1 & r_2 \end{smallmatrix}; \tau \right] = i\pi (k-1)! (X_1 - \tau Y_1)^{r_1} (X_2 - \tau Y_2)^{r_2} \Delta_k(\tau) d\tau, \quad r_1 + r_2 = k-2. \quad (4.52)$$

This equivariant $(1, 0)$ -form may be viewed as the cuspidal analogue of $\mathbb{G}_k[X, Y; \tau]$ in (4.40), where (X, Y) is split into two pairs (X_i, Y_i) with partial homogeneity degrees r_i . The

simplest non-vanishing examples of $f_{k_1, k_2}^0(\tau)$ and $\overline{g_{k_1, k_2}^0(\tau)}$ are

$$\begin{aligned}
 (f_{4,10}^0(\tau), \overline{g_{4,10}^0(\tau)}) &= -\frac{1}{2700 \cdot 11!} \frac{\Lambda(\Delta_{12}, 12)}{\Lambda(\Delta_{12}, 10)} \left(\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_2 \end{bmatrix}; \tau, -\overline{\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_2 \end{bmatrix}; \tau} \right), \\
 (f_{6,8}^0(\tau), \overline{g_{6,8}^0(\tau)}) &= \frac{1}{4200 \cdot 11!} \frac{\Lambda(\Delta_{12}, 12)}{\Lambda(\Delta_{12}, 10)} \left(\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_4 & Y_6 \end{bmatrix}; \tau, -\overline{\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_4 & Y_6 \end{bmatrix}; \tau} \right), \\
 (f_{4,12}^0(\tau), \overline{g_{4,12}^0(\tau)}) &= -\frac{1}{1382 \cdot 11!} \frac{\Lambda(\Delta_{12}, 13)}{\Lambda(\Delta_{12}, 11)} \frac{(X_1 Y_2 - X_2 Y_1)}{(i\pi)} \left(\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_9 \end{bmatrix}; \tau, \overline{\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_9 \end{bmatrix}; \tau} \right), \\
 (f_{6,10}^0(\tau), \overline{g_{6,10}^0(\tau)}) &= \frac{5}{8292 \cdot 11!} \frac{\Lambda(\Delta_{12}, 13)}{\Lambda(\Delta_{12}, 11)} \frac{(X_1 Y_2 - X_2 Y_1)}{(i\pi)} \left(\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_7 \end{bmatrix}; \tau, \overline{\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_7 \end{bmatrix}; \tau} \right), \\
 (f_{8,8}^0(\tau), \overline{g_{8,8}^0(\tau)}) &= -\frac{3}{5528 \cdot 11!} \frac{\Lambda(\Delta_{12}, 13)}{\Lambda(\Delta_{12}, 11)} \frac{(X_1 Y_2 - X_2 Y_1)}{(i\pi)} \left(\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_5 & Y_5 \end{bmatrix}; \tau, \overline{\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_5 & Y_5 \end{bmatrix}; \tau} \right).
 \end{aligned} \tag{4.53}$$

Starting from $k_1 + k_2 = 18$, generic $f_{k_1, k_2}^0(\tau)$ and $\overline{g_{k_1, k_2}^0(\tau)}$ comprise several cusp forms,

$$\begin{aligned}
 (f_{8,10}^0(\tau), \overline{g_{8,10}^0(\tau)}) &= -\frac{1}{7840 \cdot 15!} \frac{\Lambda(\Delta_{16}, 16)}{\Lambda(\Delta_{16}, 14)} \left(\Delta_{16} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_8 \end{bmatrix}; \tau, -\overline{\Delta_{16} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_8 \end{bmatrix}; \tau} \right) \\
 &\quad - \frac{1}{1560 \cdot 11!} \frac{\Lambda(\Delta_{12}, 14)}{\Lambda(\Delta_{12}, 10)} \frac{(X_1 Y_2 - X_2 Y_1)^2}{(i\pi)^2} \left(\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_6 \end{bmatrix}; \tau, -\overline{\Delta_{12} \begin{bmatrix} X_1 & X_2 \\ Y_1 & Y_6 \end{bmatrix}; \tau} \right),
 \end{aligned} \tag{4.54}$$

and the relative sign between Δ_k and $\overline{\Delta_k}$ in M_{k_1, k_2} is $+1$ (-1) if $\frac{1}{2}(k_1 + k_2 + k)$ is even (odd). Similar to the Eisenstein case in (4.49), the cuspidal contributions with $k_1 \leftrightarrow k_2$ interchanged can be obtained from

$$\begin{aligned}
 f_{k_1, k_2}^0[X_1, Y_1, X_2, Y_2; \tau] &= -f_{k_2, k_1}^0[X_2, Y_2, X_1, Y_1; \tau], \\
 \overline{g_{k_1, k_2}^0[X_1, Y_1, X_2, Y_2; \tau]} &= -\overline{g_{k_2, k_1}^0[X_2, Y_2, X_1, Y_1; \tau]}.
 \end{aligned} \tag{4.55}$$

The coefficients of Δ_k and $\overline{\Delta_k}$ are always $\mathbb{Q}[(X_1 Y_2 - X_2 Y_1)/(i\pi)]$ -linear combinations of $\zeta_{k_1, k_2}^{\Delta_k}$ in (3.28) and (3.31), with $\frac{1}{2}(k_1 + k_2 - k) - 1$ powers of $(X_1 Y_2 - X_2 Y_1)/(i\pi)$.

The integrals over $f_{k_1, k_2}^0(\tau)$ and $\overline{g_{k_1, k_2}^0(\tau)}$ exemplified in this section generate the cusp-form contributions (3.28) to depth-two β^{eqv} in (4.47). In contrast to the derivation-valued generating series J^{eqv} of modular forms β^{eqv} in (3.27), the equivariant double integrals M_{k_1, k_2} in (4.46) retain the integrals of holomorphic cusp forms. One can equivalently generalize J^{eqv} by re-interpreting the $\epsilon_k^{(j)}$ at $k \geq 4$ and $0 \leq j \leq k-2$ as generators of a free algebra rather than brackets of Tsunogai's derivations and thereby preventing the dropouts of modular forms due to relations among commutators of $\epsilon_k^{(j)}$. This viewpoint is taken in intermediate steps to motivate (3.22) as a generating series of *all* the $\alpha_{\text{hard}} \begin{bmatrix} j_1 & j_2 \\ k_1 & k_2 \end{bmatrix}; \tau$, without any dropouts. Based on the combinations M_{k_1, k_2, k_3} of β^{eqv} at depth three in upcoming work [45], the same logic applies to the generating series (B.10) of $\alpha_{\text{hard}} \begin{bmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{bmatrix}; \tau$.

5 Conclusions and further directions

In this work, we have established a dictionary between Brown's non-holomorphic modular forms obtained from equivariant iterated Eisenstein integrals (EIEIs) and the modular graph forms (MGFs) in the low-energy expansion of one-loop closed-string amplitudes. In spite of

rapid progress in representing MGFs via iterated Eisenstein integrals and their complex conjugates [42, 43, 65, 67], it was a long-standing problem to pinpoint their connection to Brown’s EIEIs [35–37]. Based on new structural results on the building blocks of MGFs with detailed studies at depths two and three, see section 3, we spell out their explicit relations with the key quantities of Brown’s construction in section 4.

One central ingredient of Brown’s EIEIs is a change of alphabet ϕ^{sv} for Tsunogai’s derivations ϵ_k that appear as non-commutative bookkeeping variables in the integration kernels. We extract an all-order expression for $\phi^{\text{sv}}(\epsilon_k)$ as an infinite series of derivations with single-valued MZVs in their coefficients from the implicit characterization of ϕ^{sv} in [35, 37]. This series-representation of $\phi^{\text{sv}}(\epsilon_k)$ involves nested commutators of ϵ_k with additional derivations z_3, z_5, \dots studied in the mathematics literature. While the depth-two parts of $[z_m, \epsilon_k]$ are known from Hain and Matsumoto [55], we provide the higher-depth completions for a variety of such commutators beyond the examples in [53].

Our new results on the derivation algebra, as well as a variety of examples for other quantities of interest in this work, can be found in the supplementary material attached to this paper. A longer follow-up paper [45] will elaborate on intermediate steps and extensions of our results, including

- depth-three analogues of the solutions $F_{m,k}^{\pm(s)}$ to Laplace eigenvalue equations at depth two [43] that were used in the derivation of some of our results
- double integrals mixing holomorphic Eisenstein series and cusp forms that were studied from a Poincaré-series perspective in [78] and enter our modular integrals at depth three
- depth-three analogues of Brown’s equivariant double iterated integrals (4.46) as well as their cocycles and $\text{SL}(2, \mathbb{R})$ multiplet structure

Apart from building a bridge between the mathematics and physics literature on non-holomorphic modular forms, this work stimulates numerous research lines for the future:

First, Brown’s construction of purely τ -dependent non-holomorphic modular forms calls for an extension to so-called elliptic modular graph forms [79, 80] which additionally depend on marked points z on a torus. Elliptic modular graph forms extend Zagier’s single-valued elliptic polylogarithms [81] to higher depth and were recently translated into z -dependent analogues of the real-analytic iterated integrals β^{sv} for conventional modular graph forms [82]. The dictionary between β^{sv} and EIEIs established in this work should guide the construction of similar generating functions of elliptic modular graph forms that manifest their (anti-)meromorphic iterated-integral constituents.

Second, it would be interesting to revisit the proposal [67] of MGFs being single-valued versions of elliptic MZVs in the light of this work: by relating MGFs with Brown’s single-valued iterated Eisenstein integrals, our results pave the way to compare the proposal in the reference with the general frameworks of single-valued integration [63, 83] and single-valued periods [64, 84]. This kind of follow-up study aims to extract information on loop amplitudes of closed strings from single-valued open-string data.

Third, the variety of perspectives obtained on MGFs at genus one is expected to inspire the study of higher-genus modular graph forms [79, 85] and tensors [86]. The quest for the algebraic [86, 87] and differential [88–90] relations of higher-genus modular graph forms might greatly benefit from an organizing principle based on iterated primitives of meromorphic modular tensors. The description of genus-one MGFs via iterated Eisenstein integrals in this work is hoped to find an echo at higher genus.

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A Explicit formula for $\overline{\alpha_{\text{hard}}}$ at depth two

In this appendix, we reformulate the all-order solution for the $\overline{\alpha_{\text{hard}}}$ at depth two in (3.21) as an explicit formula instead of a generating-series identity (3.22). By inserting the commutators (3.23) into the generating series and treating all the $\epsilon_{k_1}^{(j_1)}\epsilon_{k_2}^{(j_2)}$ as independent, one can solve for

$$\begin{aligned} \overline{\alpha_{\text{hard}} \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} ; \tau \right]} &= \theta(k_1 > k_2)\theta(k_2-2 \leq j_1+j_2 \leq k_1-2)\sigma \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix} ; \tau \right] \\ &\quad - \theta(k_2 > k_1)\theta(k_1-2 \leq j_1+j_2 \leq k_2-2)\sigma \left[\begin{matrix} j_2 & j_1 \\ k_2 & k_1 \end{matrix} ; \tau \right], \end{aligned} \tag{A.1}$$

where the $\theta(\dots)$ are taken to be 1 if the inequalities in the bracket hold and zero otherwise. Moreover, we have introduced the shorthand

$$\overline{\sigma \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} = \tag{A.2}$$

$$\frac{2\zeta_{k_2-1}(k_1-k_2+1)(k_1-k_2+2)!(k_2-j_2-2)!(k_1-j_1-2)!B_{k_1}}{(k_2-1)k_1!(k_1-1)!B_{k_1-k_2+2}}$$

$$\times (j_1+j_2-k_2+2)! \overline{\mathcal{E}_0(k_1-k_2+2, 0^{j_1+j_2-k_2+2}; \tau)} \sum_{\ell=\max(0, j_1-k_1+k_2)}^{k_2-j_2-2} \frac{(-1)^\ell (k_1-k_2+\ell)!}{\ell!(k_2-j_2-2-\ell)!(\ell-j_1+k_1-k_2)!}$$

for the antiholomorphic T -invariants $\overline{\mathcal{E}_0}$ defined in (3.19).

B Antiholomorphic T -invariants $\overline{\alpha}$ at depth three

This appendix provides a conjectural all-order expression for the $\overline{\alpha \left[\begin{matrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{matrix}; \tau \right]}$ at depth three that resembles (3.21) for $\overline{\alpha \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]}$ at depth two. The subsequent depth-three results were crucial to guide us towards a matching of the two generating series (4.2) and (4.26) of modular forms β^{equiv} . It will be convenient to represent the T -invariants (3.19) entering the $\overline{\alpha \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]}$ via

$$\overline{\mathcal{E}_0 \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau \right]} = j_1! \overline{\mathcal{E}_0(k_1, 0^{j_1}; \tau)}. \tag{B.1}$$

Moreover, the expressions in this appendix involve their generalization

$$\overline{\mathcal{E}_0 \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} = j_2! \sum_{r=0}^{j_2} \frac{(j_1+r)!}{r!} \overline{\mathcal{E}_0(k_2, 0^{j_2-r}, k_1, 0^{j_1+r}; \tau)} \tag{B.2}$$

$$+ \frac{(j_1+j_2+1)! B_{k_1}}{k_1!(j_1+1)} \overline{\mathcal{E}_0(k_2, 0^{j_1+j_2+1}; \tau)} - \frac{(j_1+j_2+1)! B_{k_2}}{k_2!(j_2+1)} \overline{\mathcal{E}_0(k_1, 0^{j_1+j_2+1}; \tau)},$$

where the first line of the right-hand side features double integrals of the T -invariant kernels $G_k^0(\tau) = G_k(\tau) - 2\zeta_k = O(q)$ [66]:

$$\mathcal{E}_0(k_1, 0^{p_1}, k_2, 0^{p_2}; \tau) = \frac{(2\pi i)^{p_1+p_2-k_1-k_2+2}}{p_1! p_2!} \int_{\tau}^{i\infty} d\tau_2 (\tau-\tau_2)^{p_2} G_{k_2}^0(\tau_2) \int_{\tau_2}^{i\infty} d\tau_1 (\tau_2-\tau_1)^{p_1} G_{k_1}^0(\tau_1)$$

$$= \frac{4}{(k_1-1)!(k_2-1)!} \sum_{m_1, n_1, m_2, n_2=1}^{\infty} \frac{m_1^{k_1-1} m_2^{k_2-1} q^{m_1 n_1 + m_2 n_2}}{(m_1 n_1)^{p_1+1} (m_1 n_1 + m_2 n_2)^{p_2+1}}. \tag{B.3}$$

As will be detailed in section B.3 below, the antiholomorphic T -invariants in (B.1) and (B.2) are related via shuffle relations

$$\overline{\mathcal{E}_0 \left[\begin{matrix} j_1 \\ k_1 \end{matrix}; \tau \right]} \overline{\mathcal{E}_0 \left[\begin{matrix} j_2 \\ k_2 \end{matrix}; \tau \right]} = \overline{\mathcal{E}_0 \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} + \overline{\mathcal{E}_0 \left[\begin{matrix} j_2 & j_1 \\ k_2 & k_1 \end{matrix}; \tau \right]} \tag{B.4}$$

and can be rewritten in terms of Brown's iterated Eisenstein integrals over kernels $\overline{\tau^j G_k(\tau)}$ with $0 \leq j \leq k-2$ and powers of $2\pi i \bar{\tau}$ as coefficients. More specifically, the results of

section B.3 imply the following alternative formula for $\overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]}$ which generalizes (3.20) for $\overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}; \tau \right]}$

$$\begin{aligned} \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]} &= \sum_{\ell_1=0}^{k_1-2-j_1} \sum_{\ell_2=0}^{k_2-2-j_2} \frac{\binom{k_1-2-j_1}{\ell_1} \binom{k_2-2-j_2}{\ell_2}}{(-4y)^{\ell_1+\ell_2}} \beta_- \left[\begin{smallmatrix} j_2+\ell_2 & j_1+\ell_1 \\ k_2 & k_1 \end{smallmatrix}; \tau \right] \\ &\quad - \frac{\mathbf{B}_{k_2} (-2\pi i \bar{\tau})^{j_2+1}}{(j_2+1)k_2!} \sum_{\ell_1=0}^{k_1-2-j_1} \frac{\binom{k_1-2-j_1}{\ell_1}}{(-4y)^{\ell_1}} \beta_- \left[\begin{smallmatrix} j_1+\ell_1 \\ k_1 \end{smallmatrix}; \tau \right] + \frac{\mathbf{B}_{k_1} \mathbf{B}_{k_2} (-2\pi i \bar{\tau})^{j_1+j_2+2}}{(j_2+1)(j_1+j_2+2)k_1!k_2!}. \end{aligned} \quad (\text{B.5})$$

Similar to (3.21), we shall split the desired T -invariants into two parts

$$\overline{\alpha \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}; \tau \right]} = \overline{\alpha_{\text{easy}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}; \tau \right]} + \overline{\alpha_{\text{hard}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}; \tau \right]}, \quad (\text{B.6})$$

and discuss the construction of $\overline{\alpha_{\text{easy}}}$ and $\overline{\alpha_{\text{hard}}}$ separately in the next two subsections. We have checked that all the $\overline{\alpha[\dots; \tau]}$ with $k_1+k_2+k_3 \leq 20$ and $0 \leq j_i \leq k_i-2$ obtained from a depth-three generalization of $\mathbb{F}_{m,k}^{\pm(s)}$ [45] are reproduced by (B.6) with the $\overline{\alpha_{\text{easy}}}$ and $\overline{\alpha_{\text{hard}}}$ below. Our results are consistent with the necessary condition

$$\overline{\alpha \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}; \tau \right]} + \overline{\alpha \left[\begin{smallmatrix} j_2 & j_1 & j_3 \\ k_2 & k_1 & k_3 \end{smallmatrix}; \tau \right]} + \overline{\alpha \left[\begin{smallmatrix} j_2 & j_3 & j_1 \\ k_2 & k_3 & k_1 \end{smallmatrix}; \tau \right]} = 0 \quad (\text{B.7})$$

for the shuffle relations (3.13) of the β^{sv} at depth three.

B.1 $\overline{\alpha_{\text{easy}}}$ at depth three

The first part of (B.6) dubbed $\overline{\alpha_{\text{easy}}}$ is determined by the c^{sv} at depth ≤ 2 multiplied by the above $\overline{\mathcal{E}_0}$ as well as the $\overline{\alpha_{\text{hard}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]}$ of appendix A,

$$\begin{aligned} \overline{\alpha_{\text{easy}} \left[\begin{smallmatrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{smallmatrix}; \tau \right]} &= \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix} \right] + \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_3 & j_2 \\ k_3 & k_2 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix} \right] - \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}; \tau \right]} \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix} \right] \\ &\quad + \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_3 \\ k_2 & k_3 \end{smallmatrix} \right] + \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix} \right] - \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix} \right] c^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix} \right] \\ &\quad + c^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix} \right] \overline{\alpha_{\text{hard}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]} - c^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix} \right] \overline{\alpha_{\text{hard}} \left[\begin{smallmatrix} j_2 & j_3 \\ k_2 & k_3 \end{smallmatrix}; \tau \right]}. \end{aligned} \quad (\text{B.8})$$

At leading depth of the respective β_- in (3.20) and (B.5), the conversion of (B.8) to $\overline{\kappa[\dots; \tau]}$ via (2.16) reproduces the first three lines of (4.35). In particular, the contributions of $\overline{\alpha_{\text{hard}}}$ to (B.8) line up with the terms $\delta_\phi \beta_- \left[\begin{smallmatrix} j_2 & j_1 \\ k_2 & k_1 \end{smallmatrix} \right] d^{\text{sv}} \left[\begin{smallmatrix} j_3 \\ k_3 \end{smallmatrix} \right] - d^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix} \right] \delta_\phi \beta_- \left[\begin{smallmatrix} j_3 & j_2 \\ k_3 & k_2 \end{smallmatrix} \right]$ in the third line of (4.35). Note that the first two lines of (B.8) intuitively generalize the rewriting

$$\overline{\alpha_{\text{easy}} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]} = \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix} \right] - \overline{\mathcal{E}_0 \left[\begin{smallmatrix} j_2 \\ k_2 \end{smallmatrix}; \tau \right]} c^{\text{sv}} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix} \right] \quad (\text{B.9})$$

of the $\overline{\alpha_{\text{easy}}}$ at depth two in (3.21).

B.2 $\overline{\alpha_{\text{hard}}}$ at depth three

Similar to (3.22), the $\overline{\alpha_{\text{hard}}}$ at depth three are most conveniently encoded in generating series (see the supplementary material for the $[z_{2m+1}, \epsilon_k]$ on the right-hand side),

$$\begin{aligned}
 & \sum_{k_1, k_2, k_3=4}^{\infty} \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \sum_{j_3=0}^{k_3-2} \frac{(k_1-1)(k_2-1)(k_3-1)(-1)^{j_1+j_2+j_3}}{(k_1-j_1-2)!(k_2-j_2-2)!(k_3-j_3-2)!} \\
 & \quad \times \overline{\alpha_{\text{hard}} \left[\begin{matrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{matrix}; \tau \right]} \epsilon_{k_3}^{(k_3-j_3-2)} \epsilon_{k_2}^{(k_2-j_2-2)} \epsilon_{k_1}^{(k_1-j_1-2)} \\
 & = \sum_{m=1}^{\infty} 2\zeta_{2m+1} \sum_{k=4}^{\infty} \sum_{j=0}^{k-2} \frac{(k-1)(-1)^j}{(k-j-2)!} \overline{\mathcal{E}_0 \left[\begin{matrix} j \\ k \end{matrix}; \tau \right]} [z_{2m+1}, \epsilon_k^{(k-j-2)}] \Big|_{\text{depth } 3} \\
 & + \sum_{m_1, m_2=1}^{\infty} 2\zeta_{2m_1+1} \zeta_{2m_2+1} \sum_{k=4}^{\infty} \sum_{j=0}^{k-2} \frac{(k-1)(-1)^j}{(k-j-2)!} \\
 & \quad \times \overline{\mathcal{E}_0 \left[\begin{matrix} j \\ k \end{matrix}; \tau \right]} [z_{2m_1+1}, [z_{2m_2+1}, \epsilon_k^{(k-j-2)}]] \Big|_{\text{depth } 3} \\
 & + \sum_{m=1}^{\infty} 2\zeta_{2m+1} \sum_{k_1, k_2=4}^{\infty} \sum_{j_1=0}^{k_1-2} \sum_{j_2=0}^{k_2-2} \frac{(k_1-1)(k_2-1)(-1)^{j_1+j_2}}{(k_1-j_1-2)!(k_2-j_2-2)!} \\
 & \quad \times \overline{\mathcal{E}_0 \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]} [[z_{2m+1}, \epsilon_{k_2}^{(k_2-j_2-2)}] \Big|_{\text{depth } 2}, \epsilon_{k_1}^{(k_1-j_1-2)}] .
 \end{aligned} \tag{B.10}$$

The $\overline{\mathcal{E}_0 \left[\begin{matrix} j \\ k \end{matrix}; \tau \right]}$ on the right-hand side contribute β_- of depth one via (3.20) which match the $\delta_\phi \beta_- \left[\begin{matrix} j_3 & j_2 & j_1 \\ k_3 & k_2 & k_1 \end{matrix}; \tau \right] \Big|_{\text{depth } 1}$ in the fourth line of (4.35) (again after conversion (2.16) to $\kappa[\dots; \tau]$). The nested brackets in the last two lines of (B.10) reproduce the contributions $\delta_\phi \beta_- \left[\begin{matrix} j_3 & j_2 & j_1 \\ k_3 & k_2 & k_1 \end{matrix}; \tau \right] \Big|_{\text{depth } 2} - \delta_\phi \beta_- \left[\begin{matrix} j_2 & j_1 \\ k_2 & k_1 \end{matrix}; \tau \right] \beta_- \left[\begin{matrix} j_3 \\ k_3 \end{matrix}; \tau \right]$ in the fourth line of (4.35) when the $\mathcal{E}_0 \left[\begin{matrix} j_1 & j_2 \\ k_1 & k_2 \end{matrix}; \tau \right]$ are restricted to the β_- of depth two in (B.5). Finally, the last line of (4.35) has depth zero as well as at least one power of $\bar{\tau}$ in each term and should account for the contributions to (3.20) and (B.5) without any factor of β_- .

Similar to the comments before section 3.4, the coefficients of $\epsilon_{k_1}^{(j_1)} \epsilon_{k_2}^{(j_2)} \epsilon_{k_3}^{(j_3)}$ in the generating-series identity (B.10) are understood to be equated before employing any commutator relation in Tsunogai's derivation algebra. The $\overline{\alpha_{\text{hard}} \left[\begin{matrix} j_1 & j_2 & j_3 \\ k_1 & k_2 & k_3 \end{matrix}; \tau \right]}$ are defined individually from (B.10) when the commutators among z_m and ϵ_k are evaluated through (3.23) and the expressions in the supplementary material.

B.3 \mathcal{E}_0 at depth two from iterated integrals

We conclude this appendix by elaborating on the origin of the antiholomorphic T -invariants at depth two in (B.2) from iterated integrals over kernels $G_k^0(\tau) = G_k(\tau) - 2\zeta_k = O(q)$. The first line of (B.2) can be traced back to

$$\begin{aligned}
 & (2\pi i)^{2+j_1+j_2-k_1-k_2} \int_{\bar{\tau}}^{-i\infty} d\bar{\tau}_1 (\bar{\tau}_1 - \bar{\tau})^{j_1} \overline{G_{k_1}^0(\tau_1)} \int_{\bar{\tau}_1}^{-i\infty} d\bar{\tau}_2 (\bar{\tau}_2 - \bar{\tau})^{j_2} \overline{G_{k_2}^0(\tau_2)} \\
 & = (2\pi i)^{2+j_1+j_2-k_1-k_2} \sum_{r=0}^{j_2} \binom{j_2}{r} \int_{\bar{\tau}}^{-i\infty} d\bar{\tau}_1 (\bar{\tau}_1 - \bar{\tau})^{j_1+r} \overline{G_{k_1}^0(\tau_1)} \int_{\bar{\tau}_1}^{-i\infty} d\bar{\tau}_2 (\bar{\tau}_2 - \bar{\tau}_1)^{j_2-r} \overline{G_{k_2}^0(\tau_2)} \\
 & = j_2! \sum_{r=0}^{j_2} \frac{(j_1+r)!}{r!} \overline{\mathcal{E}_0(k_2, 0^{j_2-r}, k_1, 0^{j_1+r}; \tau)},
 \end{aligned} \tag{B.11}$$

where we have rewritten $(\bar{\tau}_2 - \bar{\tau})^{j_2} = \sum_{r=0}^{j_2} \binom{j_2}{r} (\bar{\tau}_1 - \bar{\tau})^r (\bar{\tau}_2 - \bar{\tau}_1)^{j_2 - r}$ and identified the $\overline{\mathcal{E}_0}$ through their iterated-integral representation in (B.3). By comparing with the integral representation (3.19) of $\overline{\mathcal{E}_0} \left[\begin{smallmatrix} j \\ k \end{smallmatrix}; \tau \right]$, already the restriction of $\overline{\mathcal{E}_0} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]$ to the double integrals (B.11) is easily seen to obey the shuffle relation (B.4). The second line of (B.2) involving depth-one integrals over $G_{k_i}^0$ in turn is antisymmetric under $(j_1, k_1) \leftrightarrow (j_2, k_2)$ and therefore drops out from the symmetrized combination on the right-hand side of the shuffle relation (B.4). Hence, the shuffle property of the $\overline{\mathcal{E}_0}[\dots; \tau]$ is a consequence of the integral representation (B.11).

We shall now state an alternative integral representation of the $\overline{\mathcal{E}_0} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right]$ which manifests their relation with Brown's kernels $\bar{\tau}^j \overline{G_k(\tau)}$ with $0 \leq j \leq k-2$: following the tangential-basepoint regularization of [35], one can retrieve (B.2) from

$$\begin{aligned} \overline{\mathcal{E}_0} \left[\begin{smallmatrix} j_1 & j_2 \\ k_1 & k_2 \end{smallmatrix}; \tau \right] &= (2\pi i)^{2+j_1+j_2-k_1-k_2} \int_{\bar{\tau}}^{-i\infty} d\bar{\tau}_1 (\bar{\tau}_1 - \bar{\tau})^{j_1} \overline{G_{k_1}(\tau_1)} \int_{\bar{\tau}_1}^{-i\infty} d\bar{\tau}_2 (\bar{\tau}_2 - \bar{\tau})^{j_2} \overline{G_{k_2}(\tau_2)} \\ &\quad - \frac{B_{k_2} (-2\pi i \bar{\tau})^{j_2+1}}{(j_2+1)k_2!} \overline{\mathcal{E}_0} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}; \tau \right] - \frac{B_{k_1} B_{k_2} (-2\pi i \bar{\tau})^{j_1+j_2+2}}{(j_1+1)(j_1+j_2+2)k_1!k_2!}. \end{aligned} \tag{B.12}$$

Each term on the right-hand side is an (iterated) integral of kernels $\bar{\tau}_i^{j_i} \overline{G_{k_i}(\tau_i)}$ with $0 \leq j_i \leq k_i - 2$ with $\mathbb{Q}[2\pi i \bar{\tau}]$ -coefficients: this is evidently the case for the first line of (B.12) upon binomial expansion of both factors of $(\bar{\tau}_i - \bar{\tau})^{j_i}$, and the depth-one term $\overline{\mathcal{E}_0} \left[\begin{smallmatrix} j_1 \\ k_1 \end{smallmatrix}; \tau \right]$ in the second line can be checked to have the same property via binomial expansion in (3.19). The alternative form (B.5) in terms of β_- follows from rearranging the integral in the first line of (B.12) and applying (3.20) to its second line.

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