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Canonicalizing zeta generators: genus zero and genus one

Daniele Dorigoni[1], Mehregan Doroudiani[2], Joshua Drewitt[3], Martijn Hidding[4,5], Axel Kleinschmidt[2,6], Oliver Schlotterer[4], Leila Schneps[7] and Bram Verbeek[4]

[1] *Centre for Particle Theory & Department of Mathematical Sciences Durham University, Lower Mountjoy, Stockton Road, Durham DH1 3LE, UK*

[2] *Max-Planck-Institut für Gravitationsphysik (Albert-Einstein-Institut) Am Mühlenberg 1, 14476 Potsdam, Germany*

[3] *School of Mathematics, University of Bristol, Queens Road, Bristol, BS8 1QU, UK*

[4] *Department of Physics and Astronomy, Uppsala University, 75108 Uppsala, Sweden*

[5] *Institute for Theoretical Physics, ETH Zurich, 8093 Zürich, Switzerland*

[6] *International Solvay Institutes, ULB-Campus Plaine CP231, 1050 Brussels, Belgium*

[7] *CNRS, Sorbonne Université, Campus Pierre et Marie Curie 4 place Jussieu, 75005 Paris, France*

Zeta generators are derivations associated with odd Riemann zeta values that act freely on the Lie algebra of the fundamental group of Riemann surfaces with marked points. The genus-zero incarnation of zeta generators are Ihara derivations of certain Lie polynomials in two generators that can be obtained from the Drinfeld associator. We characterize a canonical choice of these polynomials, together with their non-Lie counterparts at even degrees $w \geq 2$, through the action of the dual space of formal and motivic multizeta values. Based on these canonical polynomials, we propose a canonical isomorphism that maps motivic multizeta values into the f-alphabet.
The canonical Lie polynomials from the genus-zero setup determine canonical zeta generators in genus one that act on the two generators of Enriquez' elliptic associators. Up to a single contribution at fixed degree, the zeta generators in genus one are systematically expanded in terms of Tsunogai's geometric derivations dual to holomorphic Eisenstein series, leading to a wealth of explicit high-order computations. Earlier ambiguities in defining the non-geometric part of genus-one zeta generators are resolved by imposing a new representation-theoretic condition. The tight interplay between zeta generators in genus zero and genus one unravelled in this work connects the construction of single-valued multiple polylogarithms on the sphere with iterated-Eisenstein-integral representations of modular graph forms.

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1 Introduction

In this article we set forth some canonical features of motivic multizeta values or, more precisely, of the Hopf algebra comodule $\mathcal{MZ}$ of motivic multizeta values and its graded dual, the Hopf algebra module $\mathcal{MZ}^\vee$. We present canonical zeta generators in genus zero and genus one that plays a role for instance in the construction of single-valued multiple polylogarithms on the sphere [1–4] and of modular equivariant iterated integrals of Eisenstein series [5–8] inspired by string theory scattering amplitudes [9–13]. Our results also imply a canonical map from multizeta values to the f-alphabet [14,15], a representation of $\mathcal{MZ}$ that is widely used but has eluded a canonical form until this work. The methods we present in this work are constructive.

1.1 The canonical zeta generators in genus zero

Our first main contribution is the definition of a canonical set of generators for $\mathcal{MZ}^\vee$, in the form of a family of polynomials

$$g_w(x,y) \in \mathbb{Q}\langle x,y\rangle\,, \qquad w \geq 2 \tag{1.1}$$

in two non-commutative variables satisfying three natural conditions related to the intrinsic structure of $\mathcal{MZ}$. For odd values of w, the polynomials g_w are Lie polynomials which provide a set of canonical generators for the genus zero motivic Lie algebra. This is the Lie algebra of the pro-unipotent radical of the fundamental group of the Tannakian category of mixed Tate motives unramified over $\mathbb{Z}$, which is well-known to be a free Lie algebra with one generator in each odd degree $w \geq 3$ (a result established in [16]). The key tool used to define the polynomials g_w is the *Z-map*, first introduced in [17] and explained here in section 3, which is a canonical linear isomorphism from $\mathcal{MZ}^\vee$ to $\mathcal{MZ}$, or more generally between any space of multizeta values (formal, motivic, real, mod products etc.) and its dual.

The Z-map comes from the canonical isomorphism of vector spaces

$$\mathbb{Q}\langle x,y\rangle \to \mathbb{Q}[Z(w)]\,, \tag{1.2}$$

where the space on the right-hand side is the $\mathbb{Q}$-vector space on symbols $Z(w)$ indexed by all monomials w in the letters x, y, and the isomorphism is given simply by mapping $w \mapsto Z(w)$. Identifying $\mathbb{Q}\langle x,y\rangle$ with the dual space of $\mathbb{Q}[Z(w)]$ and considering the bases of monomials

w and of symbols $Z(w)$ as dual bases makes this into an isomorphism of dual vector spaces. As such, the map $w \mapsto Z(w)$ passes to an isomorphism of dual vector spaces between any quotient of $\mathbb{Q}[Z(w)]$ and its dual space considered as a subspace of $\mathbb{Q}\langle x, y\rangle$. Imposing the linear relations between motivic multizeta values on the symbols $Z(w)$ identifies the motivic multizeta algebra $\mathcal{MZ}$ as a quotient of $\mathbb{Q}[Z(w)]$, and the Z-map thus passes to a linear isomorphism between $\mathcal{MZ}^\vee$ and $\mathcal{MZ}$.

Let $\mathfrak{mz}$ denote the quotient of $\mathcal{MZ}$ modulo the linear subspace spanned by constants, non-trivial products of multizeta values, and the motivic single zeta value $\zeta_2^{\mathfrak{m}}$. Then $\mathfrak{mz}$ inherits the structure of a Lie coalgebra from the Hopf algebra comodule structure of $\mathcal{MZ}$ (cf. section 2.2.2). Let $\mathfrak{mz}^\vee \subset \mathcal{MZ}^\vee \subset \mathbb{Q}\langle x, y\rangle$ denote its dual space, which is a Lie algebra equipped with the Ihara bracket (cf. section 3.1). Like $\mathcal{MZ}$ and $\mathcal{MZ}^\vee$, the spaces $\mathfrak{mz}$ and $\mathfrak{mz}^\vee$ are graded, with finite-dimensional graded parts for $w \geq 3$. A major structure theorem by Brown [15] has shown that $\mathfrak{mz}^\vee$ is freely generated by one depth 1 Lie polynomial in each odd homogeneous weight $w \geq 3$. The universal enveloping algebra $\mathcal{U}\mathfrak{mz}^\vee$ is freely generated by the generators of $\mathfrak{mz}^\vee$ under the Poincaré–Birkhoff–Witt multiplication, which we denote by $\diamond$; in the case where $g \in \mathfrak{mz}^\vee$ and $h \in \mathcal{U}\mathfrak{mz}^\vee$, this multiplication rule has a simple form:

$$g \diamond h = gh + D_g(h)\,, \tag{1.3}$$

where D_g is the Ihara derivation of $\mathbb{Q}\langle x, y\rangle$ defined by $D_g(x) = 0$ and $D_g(y) = [y, g]$. The space $\mathcal{MZ}^\vee$ is a module over the Hopf algebra $\mathcal{U}\mathfrak{mz}^\vee$.

Let us write $\mathfrak{mz}^\vee_{\geq 2}$ for the subspace of $\mathfrak{mz}^\vee$ spanned by Ihara brackets $\{g, h\} \coloneqq g\diamond h - h\diamond g$ of the generators; this is a canonical subspace independent of any actual choice of generators. The spaces $\mathcal{MZ}$, $\mathcal{MZ}^\vee$, $\mathfrak{mz}$, $\mathfrak{mz}^\vee$ and $\mathfrak{mz}^\vee_{\geq 2}$ are all weight-graded spaces; we write $\mathcal{MZ}_w$ etc. to indicate their graded parts of weight w, all of which are finite-dimensional. Each graded piece $\mathcal{MZ}_w$ contains a canonical *reducible* subspace $\hat{R}_w$ spanned by all weight w products of lower weight multizeta values. We write $R_w \coloneqq \hat{R}_w$ if w is odd, and if w is even we let R_w denote the subspace of $\hat{R}_w$ spanned by all products except for $(\zeta_2^{\mathfrak{m}})^{w/2}$, so that

$$\begin{cases} \hat{R}_w = R_w & \text{if } w \text{ is odd}\,, \\ \hat{R}_w = \mathbb{Q}\zeta_w^{\mathfrak{m}} \oplus R_w & \text{if } w \text{ is even}\,, \end{cases} \tag{1.4}$$

where $\zeta_w^{\mathfrak{m}}$ denotes the single zeta value in weight w. We then have $\mathfrak{mz}_w = \mathcal{MZ}_w/\hat{R}_w$ for $w \geq 3$. We further define canonical subspaces of *irreducible* multizeta values (resp. non-single irreducible multizeta values) in $\mathcal{MZ}_w$ for each weight $w \geq 2$ by setting

$$\hat{I}_w \coloneqq Z(\mathfrak{mz}^\vee_w)\,, \qquad I_w \coloneqq Z\big((\mathfrak{mz}^\vee_{\geq 2})_w\big)\,, \tag{1.5}$$

where we note that

$$\begin{cases} \hat{I}_w = I_w & \text{if } w \text{ is even}\,, \\ \hat{I}_w = \mathbb{Q}\zeta_w^{\mathfrak{m}} \oplus I_w & \text{if } w \text{ is odd}\,. \end{cases} \tag{1.6}$$

In this way, we obtain a canonical decomposition of $\mathcal{MZ}_w$ into single, irreducible and reducible parts:

$$\mathcal{MZ}_w = \mathbb{Q}\zeta_w^{\mathfrak{m}} \oplus I_w \oplus R_w \qquad \text{for all } w \geq 2. \tag{1.7}$$

Let

$$\Phi^{\mathfrak{m}}_{\mathrm{KZ}}(x,y) \in \mathbb{Q}\langle\langle x,y\rangle\rangle \otimes_{\mathbb{Q}} \mathcal{MZ} \tag{1.8}$$

denote the motivic Drinfeld associator [18, 19]. For convenience, we work with the motivic power series $\Phi^{\mathfrak{m}}(x,y) \coloneqq \Phi^{\mathfrak{m}}_{\mathrm{KZ}}(x,-y)$. Apart from the definition of the Z-map and the canonical decomposition (1.7), the main results of sections 2 and 3 are summarized by:

Theorem 1.1.1. *Write $\Phi^{\mathfrak{m}}$ in any basis adapted to the canonical decomposition (1.7), and for each $w \geq 2$, set*

$$g_w \coloneqq \Phi^{\mathfrak{m}}|_{\zeta^{\mathfrak{m}}_w}\,, \tag{1.9}$$

Then the polynomials g_w lie in $\mathcal{MZ}^\vee_w$. Equivalently, g_w can be identified (with no reference to $\Phi^{\mathfrak{m}}$) as the unique polynomial in $\mathcal{MZ}^\vee_w$ satisfying the following three properties:

(i) $\langle g_w, \zeta^{\mathfrak{m}}_w\rangle = 1$, where $\langle\cdot,\cdot\rangle$ denotes the action of $\mathcal{MZ}^\vee$ on $\mathcal{MZ}$,

(ii) g_w annihilates the reducible subspace $R_w \subset \mathcal{MZ}_w$,

(iii) $Z(g_w) \in \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus R_w$, i.e. it does not contain any irreducible multizeta values in I_w.

The g_w for odd $w \geq 3$ form a canonical set of generators for the Lie algebra $\mathfrak{mz}^\vee$, and the g_w for all $w \geq 2$ form a set of generators for the Hopf algebra module $\mathcal{MZ}^\vee$ over the Hopf algebra $\mathcal{U}\mathfrak{mz}^\vee$. More precisely, every element of $\mathcal{MZ}^\vee$ can be written uniquely as a product

$$g_{w_1} \diamond \cdots \diamond g_{w_r} \diamond g_k\,, \tag{1.10}$$

where the w_i are all odd ≥ 3 and $k \geq 2$, and the multiplication proceeds from right to left using the rule (1.3).

Remark 1.1.2. For both even and odd $w \geq 2$, the polynomials g_w are canonical since the subspaces R_w, I_w in part (ii) and (iii) of Theorem 1.1.1 are. Their simplest examples are given by $g_2 = [x,y]$ and $g_3 = [x-y,[x,y]]$, and the explicit form of all g_w with $w \leq 12$ can be found in the ancillary files of the arXiv submission of this work.

1.2 The canonical f-alphabet isomorphism

Brown proved in [14, 15] that the motivic multizeta algebra $\mathcal{MZ}$ is isomorphic to a certain Hopf algebra comodule $\mathcal{F}$, known as the f-alphabet algebra, which has a very simple structure: it is a commutative algebra under the shuffle multiplication, multiplicatively generated by all monomials in an alphabet of letters f_2 and $f_3, f_5, f_7, \ldots$ which is free apart from the unique relation that f_2 commutes with all the other letters; thus we have

$$\mathcal{F} = \mathbb{Q}[f_2] \otimes_{\mathbb{Q}} \overline{\mathcal{F}}\,, \tag{1.11}$$

where $\overline{\mathcal{F}}$ is freely generated under the shuffle multiplication by all monomials in $f_3, f_5, \ldots$. The space $\overline{\mathcal{F}}$ is a commutative Hopf algebra equipped with the shuffle multiplication and the deconcatenation coproduct, and $\mathcal{F}$ is a Hopf algebra comodule equipped with the following extension of the deconcatenation coproduct to a coaction:

$$\begin{aligned} \Delta : \mathcal{F} &\to \mathcal{F} \otimes \overline{\mathcal{F}} \,, \\ f_2^n f_{w_1} \cdots f_{w_r} &\mapsto \sum_{i=0}^{r} f_2^n f_{w_1} \cdots f_{w_i} \otimes f_{w_{i+1}} \cdots f_{w_r} \,. \end{aligned} \tag{1.12}$$

In [14, 15], Brown identified the complete family of Hopf algebra comodule isomorphisms $\mathcal{MZ} \to \mathcal{F}$ normalized by $\zeta_w^{\mathfrak{m}} \mapsto f_w$, showing that it is parametrized by rational parameters indexed by any basis of non-single irreducible multizetas. In section 4, we display a canonical choice of one such isomorphism, uniquely determined as follows.

Theorem 1.2.1. *There exists a canonical normalized Hopf algebra comodule isomorphism $\rho : \mathcal{MZ} \to \mathcal{F}$ whose definition depends only on the canonical decomposition (1.7); it is characterized by each of the two following properties, which are equivalent:*

- *ρ satisfies*
$$\rho(\xi)|_{f_w} = 0 \qquad \forall\, \xi \in I_w \,, \tag{1.13}$$
- *if $\Phi^{\mathfrak{m}}$ is written in a basis adapted to the canonical decomposition (1.7), then ρ satisfies*
$$\rho(\Phi^{\mathfrak{m}})|_{f_w} = g_w \qquad \forall\, w \geq 2 \,. \tag{1.14}$$

This choice of isomorphism ρ is canonical since the subspaces I_w and the polynomials g_w in (1.13) and (1.14) are.

1.3 The canonical zeta generators in genus one

Sections 5 to 7 are dedicated to zeta generators in genus one – derivations σ_w of the free graded Lie algebra $\mathrm{Lie}[a,b]$ associated to the pro-unipotent fundamental group of the once-punctured torus. Based on earlier work in [20–23], the action of the genus one generators σ_w on a, b is determined in section 5.4 from the genus zero polynomials g_w via (with B_n the n^{th} Bernoulli number)

$$\begin{aligned} \sigma_w(s_{12}) &= 0 \,, & \sigma_w(s_{01}) &= \big[s_{01}, g_w(s_{12}, -s_{01})\big] \,, \\ s_{12} &= [b,a] \,, & s_{01} &= -b - \sum_{n\geq 1} \frac{\mathrm{B}_n}{n!} \mathrm{ad}_a^n(b) \end{aligned} \tag{1.15}$$

together with the "extension lemma" 2.1.2 of [23] reviewed in section 5.3. In view of the canonical g_w in the defining equation (1.15), we arrive at the first canonical choice of the zeta generators σ_w in genus one at arbitrary odd $w \geq 3$.

By work of Hain–Matsumoto [21], the σ_w normalize the algebra $\mathfrak{u}$ of geometric derivations ϵ_k of $\mathrm{Lie}[a,b]$ in even degrees $k \geq 0$ (i.e. combined homogeneity degrees in a and b). In fact, upon decomposing the zeta generators σ_w into an infinite number of contributions at fixed even degree $\geq w+1$, all the terms except for certain contributions at *key degree* $2w$ lie in $\mathfrak{u}$. The terms of σ_w outside $\mathfrak{u}$ are referred to as *arithmetic parts* z_w and furnish one-dimensional representations under the $\mathfrak{sl}_2$ spanned by the Lie$[a,b]$-derivations $\epsilon_0, \epsilon_0^\vee$ and $\mathrm{h} \coloneqq [\epsilon_0, \epsilon_0^\vee]$ subject to

$$\epsilon_0(a) = b\,, \quad \epsilon_0(b) = 0\,, \quad \epsilon_0^\vee(a) = 0\,, \quad \epsilon_0^\vee(b) = a\,. \tag{1.16}$$

Even with the canonical definition of σ_w, the arithmetic derivations z_w are not entirely characterized by requiring that they form an $\mathfrak{sl}_2$ singlet and that $\sigma_w - z_w \in \mathfrak{u}$. We arrive at canonical z_w by additionally imposing that they exhaust the complete $\mathfrak{sl}_2$ singlet at key degree of σ_w. More specifically, the $\epsilon_k^{(j)} \coloneqq \mathrm{ad}_{\epsilon_0}^j(\epsilon_k)$ with $j = 0, 1, \ldots, k-2$ composing $\sigma_w - z_w$ fall into $(k-1)$-dimensional representations of $\mathfrak{sl}_2$ because of $\epsilon_k^{(k-1)} = 0$. The arithmetic derivations z_w are then uniquely defined by imposing that any nested commutator $\epsilon_k^{(j)}$ at the key degree of $\sigma_w - z_w$ belongs to $\mathfrak{sl}_2$ representations of dimension ≥ 3.

Based on mould theory, we describe a first algorithm to explicitly compute the action of σ_w on a and b degree by degree and prove the following theorem:

Theorem 1.3.1 (see Theorem 5.4.1 (iii))**.** *The genus one zeta generators σ_w are entirely determined by their parts of degree $< 2w$.*

This remarkable property of σ_w can be combined with the commutation relation [21]

$$[N, \sigma_w] = 0 \quad \text{with} \quad N \coloneqq -\epsilon_0 + \sum_{k=2}^{\infty} (2k-1) \frac{\mathrm{B}_{2k}}{(2k)!} \epsilon_{2k}\,, \tag{1.17}$$

to make σ_w computationally accessible to all degrees. By solving (1.17) for $[\epsilon_0, \sigma_w]$, it relates contributions to $\sigma_w - z_w$ with different numbers of $\epsilon_{k_i}^{(j_i)}$ factors (with $0 \leq j_i \leq k_i - 2$) to be referred to as *modular depth*.[1] On these grounds, we describe a second algorithm based on (1.17) to determine $\sigma_w - z_w$ recursively in modular depth, up to highest-weight vectors of $\mathfrak{sl}_2$ in each step which are defined to lie in the kernel of ad_{ϵ_0}. We will infer from the results of [21] that there are no highest-weight vectors beyond key degree. From the viewpoint of (1.17), it is thus sufficient to know the degree $\leq 2w$ parts (though Theorem 1.3.1 even guarantees that the complete information is available from degree $< 2w$) of σ_w. The infinity of terms at degree $\geq 2w+2$ follows from (1.17) together with representation theory of $\mathfrak{sl}_2$.

This setup leads us to present a closed all-degree formula for σ_w up to contributions in $\mathfrak{u}$ of modular depth ≥ 3 (in the ellipsis),

$$\begin{aligned} \sigma_w = z_w &- \frac{1}{(w-1)!} \epsilon_{w+1}^{(w-1)} \\ &- \frac{1}{2} \sum_{d=3}^{w-2} \frac{\mathrm{BF}_{d-1}}{\mathrm{BF}_{w-d+2}} \sum_{k=d+1}^{w-1} \mathrm{BF}_{k-d+1} \mathrm{BF}_{w-k+1} s^d(\epsilon_k, \epsilon_{w-k+d}) \end{aligned} \tag{1.18}$$

[1]The Lie algebra $\mathfrak{u}$ is not free on the $\epsilon_k^{(j)}$ but satisfies relations [24–26] that are not homogeneous in modular depth which for this reason only provides a filtration rather than a grading of $\mathfrak{u}$, see Remark 5.1.6.

$$
- \sum_{d=5}^{w} \mathrm{BF}_{d-1} s^d(\epsilon_{d-1}, \epsilon_{w+1}) - \frac{1}{2} \mathrm{BF}_{w+1} s^{w+2}(\epsilon_{w+1}, \epsilon_{w+1})
$$

$$
+ \sum_{k=w+3}^{\infty} \mathrm{BF}_k \sum_{j=0}^{w-2} \frac{(-1)^j \binom{k-2}{j}^{-1}}{j!(w-2-j)!} [\epsilon_{w+1}^{(w-2-j)}, \epsilon_k^{(j)}] + \dots ,
$$

where we employ the shorthands $\mathrm{BF}_k \coloneqq \frac{\mathrm{B}_k}{k!}$ and we define

$$
s^d(\epsilon_{k_1}, \epsilon_{k_2}) \coloneqq \frac{(d-2)!}{(k_1-2)!(k_2-2)!} \sum_{i=0}^{d-2} (-1)^i [\epsilon_{k_1}^{(k_1-2-i)}, \epsilon_{k_2}^{(k_2-d+i)}] \,. \tag{1.19}
$$

The highest-weight-vector contribution $\sim \epsilon_{w+1}^{(w-1)}$ in first line of (1.18) is well-known and is used to determine the modular-depth two terms in the third and fourth line from (1.17). The second line of (1.18) is conjectural and features highest-weight vectors $s^d(\epsilon_k, \epsilon_{w-k+d})$ in each term – they are not fixed by (1.17) and confirmed by direct computation in a large number of examples. Moreover, the $d = 3$ terms in the second line of (1.18) reproduce the closed formula of Brown [27] on depth-three terms in the terminology of the reference.

Finally, (1.17) together with the terms of modular depth d in $\sigma_w - z_w$ fix the explicit form of $[z_w, \epsilon_k] \in \mathfrak{u}$ up to and including modular depth $d + 1$. Accordingly, the closed formula (1.18) determines the terms of modular depth three beyond the well-known contributions [21]

$$
[z_w, \epsilon_k] = \frac{\mathrm{BF}_{w+k-1}}{\mathrm{BF}_k} \sum_{i=0}^{w-1} \frac{(-1)^i (k+i-2)!}{i!(w+k-3)!} [\epsilon_{w+1}^{(i)}, \epsilon_{w+k-1}^{(w-i-1)}] + \dots \tag{1.20}
$$

and we give closed formulae for $[z_3, \epsilon_k]$ and $[z_5, \epsilon_k]$ at modular depth three in section 7.4.2.

1.4 Motivation and outlook

A major motivation for our study of zeta generators stems from their relevance for periods of configuration spaces of Riemann surfaces with marked points. In genus zero, the canonical polynomials g_w take center stage in the recent reformulation [4] of the motivic coaction [28, 29, 15] and the single-valued map [1–3] of multiple polylogarithms on the sphere. The genus-one zeta generators σ_w and their interplay with geometric derivations ϵ_k unlocked a fully explicit generating-series description of non-holomorphic modular forms in a companion paper [8] to this work.

As detailed in [8], the expansion of σ_w in terms of the geometric derivations ϵ_k determines the appearance of (single-valued) multizeta values in so-called modular graph forms [9, 10] in genus-one string scattering amplitudes. At a computational level, the precise expressions for σ_w in terms of ϵ_k presented in this work are crucial for an explicit realization of Brown's construction of non-holomorphic modular forms in [5, 6] which was related to modular graph forms in [7]. At a conceptual level, the intimate connection between zeta generators in genus zero and genus one presented in section 5 leads to a unified description of the single-valued map of multiple polylogarithms in one variable and iterated Eisenstein integrals [8].

These applications of zeta generators in genus zero and genus lead us to expect that generalizations thereof to compact Riemann surfaces of arbitrary genus with any number of marked points may in fact exist. Our work sets the stage for two lines of follow-up research:

- adapting zeta generators in genus one to systematic constructions of single-valued elliptic polylogarithms pioneered by Zagier [30] in any number of variables and which were more recently approached in the framework of "elliptic modular graph forms" in the string-theory literature [31–34];
- determining higher-genus incarnations of zeta generators from degenerations of the flat connections [35–38] used for constructions of polylogarithms on Riemann surfaces of arbitrary genus and applying them to non-holomorphic modular graph forms [39–41, 31, 42] and tensors [43–46].

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2 Background on multizeta values

In this section, we review basic definitions on different types of multizeta values, their relations and their Hopf-algebraic properties.

2.1 Real and formal multizeta values

2.1.1 Real multizeta values, shuffle and stuffle multiplication

The *real multizeta values* are defined by the infinite sums

$$\zeta_{k_1,k_2,\ldots,k_r} := \sum_{1\le n_1<n_2<\ldots<n_r}^{\infty} n_1^{-k_1} n_2^{-k_2} \ldots n_r^{-k_r}, \tag{2.1}$$

where $k_1, \ldots, k_r \in \mathbb{N}$ and $k_r > 1$ in order to ensure convergence of the sum. The integers r and $\sum_{i=1}^{r} k_i$ in (2.1) are respectively referred to as the *depth* and *weight* of $\zeta_{k_1,k_2,\ldots,k_r}$. Multizeta values (MZVs) satisfy a number of algebraic relations over $\mathbb{Q}$ which we discuss further below. Let us first introduce the monomial notation

$$\zeta(x^{k_r-1}y \cdots x^{k_2-1}yx^{k_1-1}y) = \zeta_{k_1,k_2,\ldots,k_r}\,, \tag{2.2}$$

where x and y are non-commutative indeterminates and the convergence property $k_r > 1$ implies that the first letter on the left-hand side is x. We say that a non-trivial monomial in x, y is *convergent* if it begins with x and ends with y; all other monomials are *non-convergent*. We extend the notation (2.2) to the definition of the *regularized zeta values* $\zeta(w)$ for all non-convergent monomials $w = y^r v x^s$ with v convergent, by the explicit formula (established in Prop. 3.2.3 of [47])

$$\zeta(w) = \sum_{a=0}^{r}\sum_{b=0}^{s}(-1)^{a+b}\zeta(y^a ⧢ y^{r-a}vx^{s-b} ⧢ x^b)\,, \tag{2.3}$$

an expression in which all the non-convergent $\zeta(w)$ cancel out so that $\zeta(y^r v x^s)$ is expressed as a linear combination of convergent words only, and which ensures that for all pairs of (convergent or non-convergent) words u, v, the ζ-values satisfy the shuffle relation

$$\zeta(u)\zeta(v) = \zeta(u ⧢ v) = \zeta(v ⧢ u)\,, \tag{2.4}$$

where ζ is considered as a linear function on words, and we fix the values $\zeta(x) = \zeta(y) = 0$ and also $\zeta(\mathbf{1}) = 1$, where $\mathbf{1}$ in the argument denotes the empty word. We recall here that the shuffle product of monomials can be defined recursively as follows: for any monomial u, we have $\mathbf{1} ⧢ u = u ⧢ \mathbf{1} = u$, and if $u, v \neq \mathbf{1}$ we write $u = au'$ and $v = bv'$, where a and b are single letters (either x or y), and we have

$$u ⧢ v = a(u' ⧢ v) + b(u ⧢ v')\,. \tag{2.5}$$

For example, writing $\zeta_2 = \zeta(xy)$, we have

$$\zeta_2^2 = \zeta(xy)^2 = \zeta(xy \sqcup\!\sqcup\, xy) = 4\zeta(xxyy) + 2\zeta(xyxy) = 4\zeta_{1,3} + 2\zeta_{2,2}\,. \tag{2.6}$$

This multiplication rule is called the *shuffle multiplication* of real MZVs.

There is a second multiplication, restricted to a subset of words w, which arises when considering the MZVs written as infinite sums as in (2.1). Indeed, the result of multiplying two such series is itself a sum of such series, as can be seen on the first example:

$$\begin{aligned} \zeta_2^2 &= \sum_{n_1\geq 1} n_1^{-2} \sum_{n_2 \geq 1} n_2^{-2} \\ &= \sum_{n_1 > n_2 \geq 1} n_1^{-2} n_2^{-2} + \sum_{n_2 > n_1 \geq 1} n_1^{-2} n_2^{-2} + \sum_{n_1 = n_2 \geq 1} n_1^{-4} \\ &= 2\zeta_{2,2} + \zeta_4\,. \end{aligned} \tag{2.7}$$

This product, called the *stuffle product*, can be computed for any pair of words u, v ending with y, as follows. We start by defining the stuffle product $u * v$ of words ending in y. To do this, we first note that every monomial u ending in y can be rewritten in the free variables $y_i = x^{i-1}y$, with $i \geq 1$:

$$u = y_{i_1} \cdots y_{i_r}\,. \tag{2.8}$$

We stipulate that for all such monomials, we have $u * \mathbf{1} = \mathbf{1} * u = u$. Then, in the case where $u, v \neq \mathbf{1}$, we peel off the first letter of each of the two words, writing $u = y_{i_1} u'$ and $v = y_{j_1} v'$ with $u' = y_{i_2} \cdots y_{i_r}$ and $v' = y_{j_2} \cdots y_{j_r}$, and define the stuffle product by the recursive rule (first developed by Hoffman in [48])

$$u * v = y_{i_1}(u' * v) + y_{j_1}(u * v') + y_{i_1 + j_1}(u' * v')\,. \tag{2.9}$$

The stuffle product is commutative and associative on words ending in y.

Associated with the stuffle product, one can define a *stuffle regularization* $\zeta_*(w)$ of MZVs for words ending in y. For convergent words w (beginning with x and ending in y) we set $\zeta_*(w) = \zeta(w)$. The stuffle-regularized MZVs for non-convergent words ending in y are defined as follows. First we deal with $\zeta_*(y^i)$ for $i \geq 0$ by writing the generating series

$$\sum_{n\geq 0} \zeta_*(y^n) y^n := \exp\left(\sum_{n \geq 2} \frac{(-1)^{n-1}}{n} \zeta(x^{n-1}y) y^n \right), \tag{2.10}$$

leading for instance to

$$\begin{aligned} \zeta_*(\mathbf{1}) &= 1\,, \\ \zeta_*(y) &= 0\,, \\ \zeta_*(y^2) &= -\tfrac{1}{2}\zeta(xy) = -\tfrac{1}{2}\zeta_2\,, \\ \zeta_*(y^3) &= \tfrac{1}{3}\zeta(x^2y) = \tfrac{1}{3}\zeta_3\,, \end{aligned} \tag{2.11}$$

$$\zeta_*(y^4) = -\tfrac{1}{4}\zeta(x^3y) + \tfrac{1}{8}\zeta(xy)^2 = -\tfrac{1}{4}\zeta_4 + \tfrac{1}{8}\zeta_2^2\,.$$

Then for monomials $y^i v$ for a non-trivial convergent word v we define the stuffle regularization by

$$\zeta_*(y^i v) = \sum_{j=0}^{i} \zeta_*(y^j)\zeta(y^{i-j}v)\,, \tag{2.12}$$

where the notation $\zeta(y^{i-j}v)$ refers to the shuffle regularization defined in (2.3).

The stuffle-regularized zeta values $\zeta_*(u)$ defined in this way satisfy the stuffle relations

$$\zeta_*(u)\zeta_*(v) = \zeta_*(u * v) = \zeta_*(v * u) \tag{2.13}$$

for every pair of monomials u, v both ending in y as a direct consequence of their infinite sum expressions (2.1) (see the original reference [48], or for a standard reference text, see [49]). In particular the stuffle relations hold for ordinary MZVs $\zeta(u)$ and $\zeta(v)$ when u and v are convergent words; for example, we have

$$xy * xy = y_2 * y_2 = 2y_2^2 + y_4 = 2xyxy + xxxy\,, \tag{2.14}$$

which corresponds to $\zeta_2^2 = 2\zeta_{2,2} + \zeta_4$ as in (2.7) above.

The family of relations between MZVs consisting of the ("regularized") shuffle relations (2.4) for all pairs of monomials u, v and the ("regularized") stuffle relations (2.13) for all pairs of words u, v both ending in y is known as *the family of regularized double shuffle relations* on MZVs. Note that if both u and v are convergent, then since $\zeta_*(u) = \zeta(u)$ and $\zeta_*(v) = \zeta(v)$, combining (2.4) and (2.13) implies that

$$\zeta(u)\zeta(v) = \zeta(u \sqcup\!\sqcup v) = \zeta(u * v) \qquad (u, v \text{ convergent})\,. \tag{2.15}$$

2.1.2 Formal MZVs

The formal MZVs, denoted by $\zeta^{\mathfrak{f}}(w)$, are symbols which by definition satisfy only the (regularized) double shuffle relations explained above, as opposed to the real MZVs which may in theory satisfy any number of additional relations, even including the possibility of being rational numbers. Let us introduce the notation for the ring of formal MZVs.

For each $n \geq 0$, let $\mathbb{Q}_n[Z(w)]$ denote the vector space spanned by formal symbols $Z(w)$ indexed by all degree n monomials w in two non-commutative variables x and y; in particular we have $\mathbb{Q}_0[Z(w)] = \mathbb{Q}$. We set

$$\mathbb{Q}[Z(w)] \coloneqq \bigoplus_{n\geq 0} \mathbb{Q}_n[Z(w)]\,, \tag{2.16}$$

and make this vector space into a commutative $\mathbb{Q}$-algebra by equipping it with the (commutative) shuffle multiplication

$$Z(u)Z(v) = Z(u \sqcup\!\sqcup v)\,. \tag{2.17}$$

Let us introduce a second set of formal symbols $Z_*(w)$ for monomials w ending in y, by

- setting $Z_*(w) := Z(w)$ for convergent w,
- defining $Z_*(y^n)$ for $n \geq 1$ by the equation (2.10) with ζ replaced by Z,
- defining $Z_*(y^i v)$ for convergent words v by equation (2.12) with ζ replaced by Z.

Given that multiplying the symbols $Z(w)$ by the shuffle multiplication (2.17) reduces products to linear combinations, all of the new symbols $Z_*(w)$ can be expressed in terms of linear combinations of the symbols $Z(w)$.

Definition 2.1.1. Let $\mathcal{I}_{\mathcal{FZ}}$ be the ideal of the ring $\mathbb{Q}[Z(w)]$ generated by the following two families of linear combinations: on the one hand the *regularizations*

$$Z(w) - \sum_{a=0}^{r} \sum_{b=0}^{s} (-1)^{a+b} Z(y^a ш y^{r-a} v x^{s-b} ш x^b)\,, \tag{2.18}$$

for all words $w = y^r v x^s$ with v convergent (adapted from (2.3)), and on the other hand the regularized stuffles given for all pairs of monomials u and v both ending in y by

$$Z_*(u) Z_*(v) - Z_*(u * v) \tag{2.19}$$

(adapted from (2.13)). The expression (2.19) is to be computed as a linear combination of symbols $Z(w')$ where the monomials w' are all of homogeneous weight equal to the sum of the weights of u and v by (i) expanding out the right-hand term as a linear combination, (ii) replacing every occurrence of Z_* by a polynomial expression in Z using (2.10) and (2.12), (iii) using the shuffle multiplication (2.17) to express all products $Z(w')Z(w'')$ as linear combinations $Z(w' ш w'')$. Thus each of the expressions in (2.18) and (2.19) is a linear combination of fixed weight; we take them all together as the generators of the ideal $\mathcal{I}_{\mathcal{FZ}}$.

Examples. *Regularization:* the formula (2.18) above for the non-convergent word $w = yxy$ tells us to add the linear combination

$$Z(yxy) - Z(yxy) + Z(y ш xy) = Z(yxy) + 2Z(xyy) \tag{2.20}$$

to the ideal $\mathcal{I}_{\mathcal{FZ}}$.

Stuffle: Let us compute the linear combination

$$Z_*(y^2) Z_*(xy) - Z_*(y^2 * xy) \tag{2.21}$$

as a linear combination of Z-symbols using the three steps explained below (2.19). Using (2.9), we have

$$yy * xy = y_1 y_1 * y_2 = y_2 y_1 y_1 + y_1 y_2 y_1 + y_1 y_2 y_2 + y_3 y_1 + y_1 y_3 = xyyy + yxyy + yyxy + xxyy + yxxy\,, \tag{2.22}$$

so by the first step, which consists of expanding out $Z_*(yy * xy)$, (2.21) can be rewritten as

$$Z_*(yy) Z_*(xy) - Z_*(xyyy) - Z_*(yxyy) - Z_*(yyxy) - Z_*(xxyy) - Z_*(yxxy)\,. \tag{2.23}$$

In the second step we replace each Z_* by an expression in Z. For the three convergent words xy, $xyyy$ and $xxyy$ we have $Z_* = Z$; by (2.11) we have $Z_*(y) = 0$ and $Z_*(yy) = -\frac{1}{2}Z(xy)$, and finally by (2.12) we have

$$\begin{aligned}
Z_*(yxyy) &= Z(yxyy) + Z_*(y)Z(xyy) = Z(yxyy)\,, \\
Z_*(yyxy) &= Z(yyxy) + Z_*(y)Z(yxy) + Z_*(yy)Z(xy) = Z(yyxy) - \tfrac{1}{2}Z(xy)^2\,, \\
Z_*(yxxy) &= Z(yxxy) + Z_*(y)Z(xxy) = Z(yxxy)\,.
\end{aligned} \tag{2.24}$$

Plugging these into (2.23) allows us to rewrite (2.21) as

$$-\tfrac{1}{2}Z(xy)^2 - Z(xyyy) - Z(yxyy) - Z(yyxy) + \tfrac{1}{2}Z(xy)^2 - Z(xxyy) - Z(yxxy)\,. \tag{2.25}$$

If necessary we could now expand out the products of Z-symbols using the shuffle, but since they cancel out we don't need to, so in the end we add the linear combination

$$-Z(xyyy) - Z(yxyy) - Z(yyxy) - Z(xxyy) - Z(yxxy) \tag{2.26}$$

to the ideal $\mathcal{I}_{\mathcal{FZ}}$.

Remark 2.1.2. Note that by (2.17), for convergent words u and v, the relations (2.19) of $\mathcal{I}_{\mathcal{FZ}}$ are of the "shuffle=stuffle" form $Z(u \sqcup\!\sqcup v) = Z(u * v)$ since $Z_*(u) = Z(u)$ and $Z_*(v) = Z(v)$. A conjecture by Hoffman (cf. [50] which is useful for practical computations in low weight) posits that the combinations

$$Z_*(u * v) - Z(u \sqcup\!\sqcup v) \tag{2.27}$$

with both u and v convergent or $u = y$ and v convergent suffice to generate the ideal $\mathcal{I}_{\mathcal{FZ}}$.

Definition 2.1.3. Let $\mathcal{I}_{\mathcal{Z}}$ be the ideal of $\mathbb{Q}[Z(w)]$ generated by all algebraic relations between real MZVs. Since the real MZVs do satisfy the regularized double shuffle relations, we have the inclusions

$$\mathcal{I}_{\mathcal{FZ}} \subset \mathcal{I}_{\mathcal{Z}} \subset \mathbb{Q}[Z(w)]\,. \tag{2.28}$$

The space $\mathcal{FZ}$ of *formal MZVs* and the space $\mathcal{Z}$ of *real MZVs* are defined by

$$\begin{aligned}
\mathcal{FZ} &\coloneqq \mathbb{Q}[Z(w)]/\mathcal{I}_{\mathcal{FZ}}\,, \\
\mathcal{Z} &\coloneqq \mathbb{Q}[Z(w)]/\mathcal{I}_{\mathcal{Z}}\,,
\end{aligned} \tag{2.29}$$

so that there is a natural surjection

$$\mathcal{FZ} \twoheadrightarrow \mathcal{Z}\,. \tag{2.30}$$

The space $\mathcal{FZ}$ is generated by the images of the $Z(w)$ in the quotient modulo $\mathcal{I}_{\mathcal{FZ}}$, which we denote $\zeta^{\mathfrak{f}}(w)$; these formal MZVs are subject by definition only to the regularized double shuffle relations coming from Definition 2.1.1. The elements of the $\mathbb{Q}$-algebra $\mathcal{Z}$ of real MZVs are denoted by $\zeta(w)$.

The $\mathbb{Q}$-algebra $\mathcal{FZ}$ is weight-graded by definition since all of its defining relations are weight-graded, while $\mathcal{Z}$ is conjectured but of course not known to be weight-graded; if it were, this would imply that all real MZVs are transcendental. A standard conjecture asserts that the surjection (2.30) is an isomorphism.

2.1.3 The Goncharov–Brown coaction

Let $\overline{\mathcal{FZ}}$ denote the quotient of $\mathcal{FZ}$ modulo the ideal generated by $\zeta_2^{\mathfrak{f}}$. In [28, 29], Goncharov introduced a coproduct on $\overline{\mathcal{FZ}}$, which makes it into a Hopf algebra. Brown subsequently defined an extension of Goncharov's coproduct to a coaction of the Hopf algebra $\overline{\mathcal{FZ}}$ on the module $\mathcal{FZ}$ [15]; restricted from $\mathcal{FZ}$ to $\overline{\mathcal{FZ}}$ in both the argument and the result, the coaction becomes Goncharov's coproduct $\overline{\mathcal{FZ}} \to \overline{\mathcal{FZ}} \otimes \overline{\mathcal{FZ}}$.[2]

There are in fact two different versions of the Goncharov–Brown coaction, which differ from each other only by the order of the tensor factors. We denote them by

$$\begin{cases} \Delta^{GB} : \mathcal{FZ} \to \overline{\mathcal{FZ}} \otimes \mathcal{FZ}\,, \\ \Delta_{GB} : \mathcal{FZ} \to \mathcal{FZ} \otimes \overline{\mathcal{FZ}}\,. \end{cases} \tag{2.31}$$

Both versions of the coaction are used regularly in the literature, so that it is important to keep track of which one is being used at all times. In the present paper, as we will specify, the coaction Δ^{GB} is implicitly used in numerous proofs in view of its compatibility with double-shuffle theory and Hopf-algebra duals. The coaction Δ_{GB} entering explicit formulae (most notably in section 4) is used to remain coherent with the recent literature[3].

Let us describe the construction of the Goncharov–Brown coaction Δ_{GB}.

Definition 2.1.4. Let w be a convergent monomial in x and y, i.e. starting with x and ending with y. Write $w = x^{k_r-1}y \cdots x^{k_1-1}y$ to match the monomial notation of $\zeta^{\mathfrak{f}}_{k_1,\dots,k_r}$ in (2.2), and associate to it the symbol

$$I(0; 1, 0^{k_1-1}, \dots, 1, 0^{k_r-1}; 1) = \zeta^{\mathfrak{f}}_{k_1,\dots,k_r}\,. \tag{2.32}$$

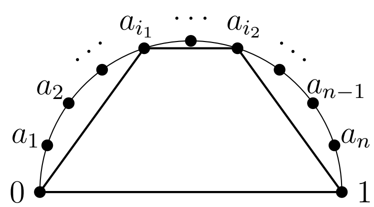
Let $n = k_1 + \cdots + k_r$ denote the degree of w. Visualize the sequence $(0; 1, 0^{k_1-1}, \dots, 1, 0^{k_r-1}; 1)$ in order from left to right around a semi-circle as illustrated in Figure 1, with the terminal 0 and 1 at the outer edges and the middle n points placed in clockwise order along the inner part of the semi-circle. To compute the coaction of the symbol $I(0; 1, 0^{k_1-1}, \dots, 1, 0^{k_r-1}; 1)$ associated with $\zeta^{\mathfrak{f}}_{k_1,\dots,k_r}$, draw every possible "polygon" inside the half-circle starting with the outer 0 on the left and ending with the outer 1 on the right, with vertices at any subset of the inner letters (including the empty set). In the notation

$$(a_1, a_2, \dots, a_n) = (1, 0^{k_1-1}, 1, 0^{k_2-1}, \dots, 1, 0^{k_r-1}) \tag{2.33}$$

for the middle n points (apart from the outer points 0 and 1), the contributing polygons are parametrized by subsets $\{a_{i_1}, a_{i_2}, \dots, a_{i_r}\}$ with $1 \le i_1 < i_2 < \cdots < i_r \le n$ and all cardinalities in the range $0 \le r \le n$; see Figure 1 for the example of $r = 2$.

[2]Strictly speaking, the definition given by Brown is only for the motivic MZVs that we introduce in section 2.2 below. It lifts without change to $\mathcal{FZ}$.

[3]The coaction Δ^{GB} based on Goncharov's original coproduct was introduced in [28, 29] and [15]. The coaction Δ_{GB} is used in the recent particle-physics, string-theory and mathematics literature such as [51–56].



$$I(0;a_{i_1},a_{i_2};1)\otimes I(0;a_1,a_2,\ldots,a_{i_1-1};a_{i_1})$$
$$\times I(a_{i_1};a_{i_1+1},\ldots,a_{i_2-1};a_{i_2})I(a_{i_2};a_{i_2+1},\ldots,a_n;1)$$

Figure 1: *Contributions to the coaction formula (2.34) for $\Delta_{GB}I(0;a_1,a_2,\ldots,a_n;1)$ from polygons with inner vertices a_{i_1},a_{i_2}, i.e. quadrilaterals associated with subsets of $a_1,a_2,\ldots,a_n$ of cardinality $r=2$.*

The coaction is computed by adding up the contributions of all possible polygons:

$$\Delta_{GB}I(0;a_1,a_2,\ldots,a_n;1)=\sum_{r=0}^{n}\sum_{1\le i_1<i_2<\ldots<i_r\le n}I(0;a_{i_1},a_{i_2},\ldots,a_{i_r};1)\otimes I(0;a_1,a_2,\ldots,a_{i_1-1};a_{i_1})$$
$$\times I(a_{i_1};a_{i_1+1},\ldots,a_{i_2-1};a_{i_2})\cdots I(a_{i_{r-1}};a_{i_{r-1}+1},\ldots,a_{i_r-1};a_{i_r})I(a_{i_r};a_{i_r+1},\ldots,a_n;1)\,, \tag{2.34}$$

where $I(0;a_{i_1},\ldots,a_{i_r};1)$ specializes to $I(0;1)=1$ in case of the empty subset at $r=0$. We simplify the expression (2.34) according to the following rules:

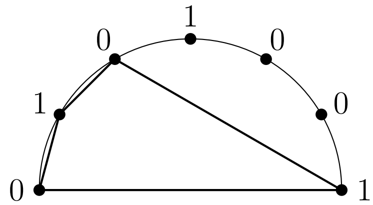
- $I(a;b)=1$ for all $a,b\in\{0,1\}$,
- $I(a;b;c)=0$ for all $a,b,c\in\{0,1\}$,
- $I(a;S;a)=0$ for $a\in\{0,1\}$ and any non-empty sequence S of $0's$ and 1's,
- $I(1;S;0)=(-1)^nI(0;\overleftarrow{S};1)$ if S is a sequence of 0's and 1's of length n and $\overleftarrow{S}$ denotes the sequence S in the reversed order.

We can also replace each term $I(0;S;1)$ by the formal (shuffle-regularized) MZV $\zeta^{\mathfrak{f}}(w_S)$, where if S is any sequence of 0's and 1's then w_S is the monomial obtained by reversing the order of S and replacing every 0 with an x and every 1 with a y. We finally project the entries of the second factor of the tensor product modulo $\zeta^{\mathfrak{f}}(xy)=\zeta_2^{\mathfrak{f}}$ to $\overline{\mathcal{FZ}}$, so that the Goncharov–Brown coaction takes values in $\mathcal{FZ}\otimes\overline{\mathcal{FZ}}$ as announced in (2.31).

Example. The coaction on the convergent word $\zeta^{\mathfrak{f}}(xxyxy)$ is computed from the semi-circle drawn in Figure 2, which shows one example of a contribution from a quadrilateral. The total result of the coaction is given by

$$\Delta_{GB}\zeta^{\mathfrak{f}}(xxyxy)=1\otimes\zeta^{\mathfrak{f}}(xxyxy)+\zeta^{\mathfrak{f}}(xxyxy)\otimes 1+3\zeta^{\mathfrak{f}}(xy)\otimes\zeta^{\mathfrak{f}}(xxy)\,. \tag{2.35}$$

The first term comes from the degenerate polygon consisting of the straight line from the outer 0 to the outer 1 with no inner vertices and the second to the full polygon touching all the inner vertices. The term with factor 3 arises from quadrilaterals involving the earliest 1 (in clockwise direction) of the type shown in Figure 2, and there are three such quadrilaterals



$$\to I(0;1,0;1) \otimes I(0;1)I(1;0)I(0;100;1)$$

$$\to \zeta^{\mathfrak{f}}(xy) \otimes \zeta^{\mathfrak{f}}(xxy)$$

Figure 2: *Example of a contribution to* $\Delta_{GB}\zeta^{\mathfrak{f}}(xxyxy)$ *as computed in* (2.35).

which produce the same non-vanishing contribution. All other polygons have a vanishing contribution; in particular the polygons going from 0 directly to the 1 at the top produce a $\zeta^{\mathfrak{f}}(xy) = \zeta_2^{\mathfrak{f}}$ to the right of the tensor product $\otimes$, which is projected to zero.

Definition 2.1.5. The coaction Δ^{GB} is obtained from Δ_{GB} by the identity

$$\Delta^{GB} = \iota \circ \Delta_{GB}\,, \tag{2.36}$$

where ι exchanges the two tensor factors

$$\begin{aligned} \iota : \mathcal{FZ} \otimes \overline{\mathcal{FZ}} &\mapsto \overline{\mathcal{FZ}} \otimes \mathcal{FZ}\,, \\ \alpha \otimes \beta &\mapsto \beta \otimes \alpha\,. \end{aligned} \tag{2.37}$$

Reducing the $\mathcal{FZ}$ factor mod $\zeta_2^{\mathfrak{f}}$ in not just one but both factors of the image yields two coproducts

$$\Delta_G, \Delta^G : \overline{\mathcal{FZ}} \to \overline{\mathcal{FZ}}\,, \tag{2.38}$$

each of which confers a Hopf algebra structure on $\overline{\mathcal{FZ}}$. We will study the Hopf algebra $\overline{\mathcal{FZ}}$ equipped with Δ^G and its dual Hopf algebra $\overline{\mathcal{FZ}}^{\vee}$ further in section 3.1.

2.2 Motivic MZVs

In this article, we will use a simplistic definition for the $\mathbb{Q}$-algebra of *motivic MZVs*, which were constructed and studied in depth as a subcategory of the category of mixed Tate motives (MTM) unramified over $\mathbb{Z}$ by Deligne, Goncharov, Manin and others, until Brown proved that the subcategory is equal to the full category (see [15]). Our definition follows from Brown's results.

2.2.1 Definition, coproduct and coaction

Definition 2.2.1. Let $\mathcal{I}_{\mathcal{MZ}}$ denote the largest ideal in $\overline{\mathcal{FZ}}$ preserved by the Goncharov coproduct Δ_G, in the sense that the coproduct passes to the quotient $\overline{\mathcal{MZ}} := \overline{\mathcal{FZ}}/\mathcal{I}_{\mathcal{MZ}}$, which thus inherits the Hopf algebra structure from $\overline{\mathcal{FZ}}$. Let $\zeta^{\mathfrak{m}}(w)$ denote the image in $\mathcal{MZ}$ of $\zeta^{\mathfrak{f}}(w) \in \overline{\mathcal{FZ}}$. Let $\mathcal{MZ}$ be the formal tensor product

$$\mathcal{MZ} = \mathbb{Q}[\zeta_2^{\mathfrak{m}}] \otimes_{\mathbb{Q}} \overline{\mathcal{MZ}}\,, \tag{2.39}$$

where $\mathbb{Q}[\zeta_2^{\mathfrak{m}}]$ denotes the polynomial ring in the symbol $\zeta_2^{\mathfrak{m}}$. The coactions Δ^{GB} and Δ_{GB} reviewed in section 2.1.3 both descend directly to $\mathcal{MZ}$. Let us review the notation for Δ_{GB}; it is identical to Δ^{GB} in (2.31) up to exchanging the two factors of the tensor product.

The descended coaction [15]

$$\Delta_{GB} : \mathcal{MZ} \to \mathcal{MZ} \otimes \overline{\mathcal{MZ}}\,, \tag{2.40}$$

makes $\mathcal{MZ}$ into a Hopf algebra comodule. In particular we have

$$\Delta_{GB}\big(\zeta_2^{\mathfrak{m}}\big) = \zeta_2^{\mathfrak{m}} \otimes 1\,. \tag{2.41}$$

In analogy with (2.32) we write $\zeta^{\mathfrak{m}}_{k_1,\ldots,k_r} = I^{\mathfrak{m}}(0;1,0^{k_1-1},\ldots,1,0^{k_r-1};1) \in \mathcal{MZ}$. We also use the notation $\zeta^{\mathfrak{dr}}_{k_1,\ldots,k_r} = I^{\mathfrak{dr}}(0;1,0^{k_1-1},\ldots,1,0^{k_r-1};1) \in \overline{\mathcal{MZ}}$ for the second tensor factor of Δ_{GB} whose reduction modulo ζ_2 translates into $\zeta_2^{\mathfrak{dr}} = 0$.[4] The explicit form of the coaction for motivic MZVs $\zeta^{\mathfrak{m}}_{k_1,\ldots,k_r}$ is encoded in symbols exactly as in (2.34): we write

$$\begin{aligned}\Delta_{GB} I^{\mathfrak{m}}(0;a_1,a_2,\ldots,a_n;1) = \sum_{r=0}^{n} \sum_{1\leq i_1<i_2<\ldots<i_r\leq n} I^{\mathfrak{m}}(0;a_{i_1},\ldots,a_{i_r};1) \otimes I^{\mathfrak{dr}}(0;a_1,\ldots,a_{i_1-1};a_{i_1})\\ \times I^{\mathfrak{dr}}(a_{i_1};a_{i_1+1},\ldots,a_{i_2-1};a_{i_2})\cdots I^{\mathfrak{dr}}(a_{i_{r-1}};a_{i_{r-1}+1},\ldots,a_{i_r-1};a_{i_r}) I^{\mathfrak{dr}}(a_{i_r};a_{i_r+1},\ldots,a_n;1)\,,\end{aligned} \tag{2.42}$$

where the rules detailed below (2.34) apply in identical form to the terms $I^{\mathfrak{m}}$ and $I^{\mathfrak{dr}}$ on the right-hand side of (2.42) and can be used to put all terms into the standard form $I^{\mathfrak{m}}(0;S;1)$ and $I^{\mathfrak{dr}}(0;S;1)$ for finite tuples S of 0's and 1's.

Examples. When $w = x^{n-1}y$ for odd values of $n = 2k+1$, the only polygons with a non-zero contribution are the degenerate one (going directly from 0 to 1) and the full polygon including every point on the semi-circle: thus we have

$$\Delta_{GB}\zeta^{\mathfrak{m}}_{2k+1} = \zeta^{\mathfrak{m}}_{2k+1} \otimes 1 + 1 \otimes \zeta^{\mathfrak{dr}}_{2k+1} \in \mathcal{MZ} \otimes \overline{\mathcal{MZ}}\,. \tag{2.43}$$

Such elements are said to be *primitive* for the coproduct. The counterparts of (2.43) for $w = x^{n-1}y$ at even $n = 2k$ simplifies to $\Delta_{GB}\zeta^{\mathfrak{m}}_{2k} = \zeta^{\mathfrak{m}}_{2k} \otimes 1$ by the vanishing of $\zeta^{\mathfrak{dr}}_{2k}$.

We also give a few other illustrative instances:

$$\begin{aligned}\Delta_{GB}(\zeta_3^{\mathfrak{m}}\zeta_5^{\mathfrak{m}}) &= \zeta_3^{\mathfrak{m}}\zeta_5^{\mathfrak{m}} \otimes 1 + 1 \otimes \zeta_3^{\mathfrak{dr}}\zeta_5^{\mathfrak{dr}} + \zeta_3^{\mathfrak{m}} \otimes \zeta_5^{\mathfrak{dr}} + \zeta_5^{\mathfrak{m}} \otimes \zeta_3^{\mathfrak{dr}}\,,\\ \Delta_{GB}(\zeta_{3,5}^{\mathfrak{m}}) &= \zeta_{3,5}^{\mathfrak{m}} \otimes 1 + 1 \otimes \zeta_{3,5}^{\mathfrak{dr}} - 5\,\zeta_3^{\mathfrak{m}} \otimes \zeta_5^{\mathfrak{dr}}\,,\\ \Delta_{GB}(\zeta_{2,6}^{\mathfrak{m}}) &= \zeta_{2,6}^{\mathfrak{m}} \otimes 1 + 1 \otimes \zeta_{2,6}^{\mathfrak{dr}} + 4\,\zeta_3^{\mathfrak{m}} \otimes \zeta_5^{\mathfrak{dr}} + 2\,\zeta_5^{\mathfrak{m}} \otimes \zeta_3^{\mathfrak{dr}}\,.\end{aligned} \tag{2.44}$$

[4]The superscript in $\zeta^{\mathfrak{dr}}$ refers to de Rham periods [29, 15, 57, 58]. In the motivic coaction Δ_{GB}, de Rham periods occur in the right entry of tensor products $A \otimes B$, i.e. B is considered modulo $i\pi$. This is opposite to the coaction Δ^{GB} of [15] where de Rham periods are in the left entry, so that (2.41) would instead read $\Delta^{GB}(\zeta_2^{\mathfrak{m}}) = 1 \otimes \zeta_2^{\mathfrak{m}}$.

These relations are compatible with

$$\zeta^{\mathfrak{m}}_{2,6} = -\frac{2}{5}\zeta^{\mathfrak{m}}_{3,5} + 2\zeta^{\mathfrak{m}}_3\zeta^{\mathfrak{m}}_5 - \frac{42}{125}(\zeta^{\mathfrak{m}}_2)^4\,, \tag{2.45}$$

where one has to use that the second entries of tensor products in $\mathcal{MZ} \otimes \overline{\mathcal{MZ}}$ are automatically projected modulo $\zeta^{\mathfrak{m}}_2$, so that $\zeta^{\mathfrak{dr}}_{2,6} = -\frac{2}{5}\zeta^{\mathfrak{dr}}_{3,5} + 2\zeta^{\mathfrak{dr}}_3\zeta^{\mathfrak{dr}}_5$.

The motivic MZVs surject down to the real MZVs by the period map

$$I^{\mathfrak{m}}(0; S; 1) \mapsto \zeta(w_S) \tag{2.46}$$

(see [15]), so we have the following sequence of $\mathbb{Q}$-algebra surjections

$$\mathcal{FZ} \twoheadrightarrow \mathcal{MZ} \twoheadrightarrow \mathcal{Z}\,, \tag{2.47}$$

with conjectured equality. Like $\mathcal{FZ}$, the Hopf algebra comodule $\mathcal{MZ}$ is graded by the weight of the MZVs, as is $\overline{\mathcal{MZ}}$. We write $\mathcal{MZ}_w$ (resp. $\overline{\mathcal{MZ}_w}$) for the weight w part of $\mathcal{MZ}$ (resp. $\overline{\mathcal{MZ}}$). Note that we have

$$\begin{aligned} \mathcal{FZ}_0 = \overline{\mathcal{FZ}_0} = \mathcal{MZ}_0 = \overline{\mathcal{MZ}_0} = \mathbb{Q}\,, \\ \mathcal{FZ}_1 = \overline{\mathcal{FZ}_1} = \mathcal{MZ}_1 = \overline{\mathcal{MZ}_1} = \{0\}\,. \end{aligned} \tag{2.48}$$

2.2.2 Reducible motivic MZVs

Let $\mathfrak{fz}$ denote the quotient of the $\mathbb{Q}$-algebra $\mathcal{FZ}$ given by

$$\mathfrak{fz} \coloneqq \mathcal{FZ}/\big(\mathcal{FZ}_0 \oplus \mathcal{FZ}_2 \oplus (\mathcal{FZ}_{>0})^2\big) = \overline{\mathcal{FZ}}/\big(\overline{\mathcal{FZ}}_0 \oplus (\overline{\mathcal{FZ}}_{>0})^2\big)\,, \tag{2.49}$$

and analogously, let $\mathfrak{mz}$ denote the quotient of the $\mathbb{Q}$-algebra $\mathcal{MZ}$ given by

$$\mathfrak{mz} \coloneqq \mathcal{MZ}/\big(\mathcal{MZ}_0 \oplus \mathcal{MZ}_2 \oplus (\mathcal{MZ}_{>0})^2\big) = \overline{\mathcal{MZ}}/\big(\overline{\mathcal{MZ}}_0 \oplus (\overline{\mathcal{MZ}}_{>0})^2\big)\,. \tag{2.50}$$

From the Hopf algebra structure on $\overline{\mathcal{FZ}}$ (resp. $\overline{\mathcal{MZ}}$), the vector space $\mathfrak{fz}$ (resp. $\mathfrak{mz}$) inherits the structure of a Lie coalgebra, dual to the Lie algebras that will be introduced in section 3.1. Note that by (2.49) and (2.50), the element $\zeta^{\mathfrak{f}}_2$ (resp. $\zeta^{\mathfrak{m}}_2$) maps down to zero in $\mathfrak{fz}$ (resp. $\mathfrak{mz}$).

Definition 2.2.2. For all even positive integers $w = 2n$, let B_{2n} be the Bernoulli number, and set

$$\zeta^{\mathfrak{m}}_{2n} \coloneqq \frac{\zeta_{2n}}{\zeta_2^n}(\zeta^{\mathfrak{m}}_2)^n = (-1)^{n-1}\frac{(24)^n\mathrm{B}_{2n}}{2(2n)!}\,(\zeta^{\mathfrak{m}}_2)^n \in \mathcal{MZ}_{2n}\,. \tag{2.51}$$

Definition 2.2.3. For all $w \geq 3$, let $\hat{R}_w$ denote the canonical subspace of *reducible MZVs* in $\mathcal{MZ}_w$. The space $\hat{R}_w$ is the subspace generated by all total-weight w products of lower-weight MZVs, or in other words by all weight w elements of $(\mathcal{MZ}_{>0})^2$. Note that $\hat{R}_3 = \{0\}$, so there are actually non-trivial reducible subspaces only for $w \geq 4$, starting with $\hat{R}_4 = \mathbb{Q}\zeta^{\mathfrak{m}}_4$ and $\hat{R}_5 = \mathbb{Q}\zeta^{\mathfrak{m}}_2\zeta^{\mathfrak{m}}_3$.

The Lie coalgebras $\mathfrak{fz}$ and $\mathfrak{mz}$ are weight-graded, and for each weight $w > 1$ we have

$$\mathfrak{fz}_w = \mathcal{FZ}_w/\hat{R}_w\,, \qquad \mathfrak{mz}_w = \mathcal{MZ}_w/\hat{R}_w\,. \tag{2.52}$$

2.2.3 Irreducible MZVs

Let $\hat{I}_w$ be any supplementary subspace of $\hat{R}_w$ in $\mathcal{MZ}_w$ so that

$$\mathcal{MZ}_w = \hat{R}_w \oplus \hat{I}_w \,. \tag{2.53}$$

Since the map $\mathcal{MZ}_w \to \mathfrak{mz}_w$ is the quotient mod $\hat{R}_w$, it induces an isomorphism $\hat{I}_w \to \mathfrak{mz}_w$. We will always choose $\hat{I}_w$ containing $\zeta^{\mathfrak{m}}_w$ if w is odd. If w is even, we set $I_w \coloneqq \hat{I}_w$, and if w is odd we choose a supplementary subspace I_w in $\hat{I}_w$ such that $\hat{I}_w = \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus I_w$. Similarly, if w is odd we set $R_w \coloneqq \hat{R}_w$ and if w is even we choose a supplementary subspace $R_w \subset \hat{R}_w$ such that $\hat{R}_w = \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus R_w$. Then for all $w \geq 2$ we have the direct sum decomposition

$$\mathcal{MZ}_w = \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus I_w \oplus R_w \,. \tag{2.54}$$

3 The Z-map associating polynomials to MZVs

In this section we will introduce the *Z-map* (see [17]), which provides a family of canonical isomorphisms between the MZV spaces studied in section 2 (namely $\mathcal{FZ}$, $\overline{\mathcal{FZ}}$, $\mathcal{MZ}$, $\overline{\mathcal{MZ}}$, $\mathcal{Z}$, $\mathfrak{fz}$ or $\mathfrak{mz}$) and their dual spaces. Since all the MZV spaces are quotients of $\mathbb{Q}[Z(w)]$, all of their duals are subspaces of $\mathbb{Q}[Z(w)]^\vee$, which is nothing other than the polynomial algebra $\mathbb{Q}\langle x, y\rangle$ in the non-commutative variables x and y.

Thanks to the fact that the double shuffle relations generate all relations satisfied by $\mathcal{FZ}$ (and in their linearized version, $\mathfrak{fz}$), we can give an explicit description of the elements of the dual spaces $\mathcal{FZ}^\vee$ and $\mathfrak{fz}^\vee$ in $\mathbb{Q}\langle x, y\rangle$. In the case of motivic and real MZVs we do not have an explicit description of this type since they may satisfy further, unknown relations. Still, thanks to Brown's theorem in [15], we do know the structure and dimensions of the graded parts of the dual spaces $\mathcal{MZ}^\vee$ and $\mathfrak{mz}^\vee$, which allows us to compute their elements explicitly in low weights (see section 3.4).

3.1 The double shuffle dual space of formal MZVs

Let $\mathbb{Q}\langle x, y\rangle$ denote the polynomial ring in two non-commutative variables x and y, equipped with its canonical basis of monomials w in x and y (including the constant monomial $\mathbf{1}$), and let $\mathbb{Q}\langle\langle x, y\rangle\rangle$ denote its degree-completion, the power series ring in x and y. The space $\mathbb{Q}[Z(w)]$ introduced in section 2.1.2 can be identified with the graded dual of $\mathbb{Q}\langle x, y\rangle$, equipped with the dual basis of symbols $Z(w)$ such that

$$\langle Z(u), v\rangle = \delta_{u,v} \,, \tag{3.1}$$

on monomials u and v and extended linearly to give a canonical pairing between $\mathbb{Q}\langle x, y\rangle$ and $\mathbb{Q}[Z(w)]$.

Recall from (2.29) that $\mathcal{FZ}$ is the quotient of $\mathbb{Q}[Z(w)]$ by the ideal $\mathcal{I}_{\mathcal{FZ}}$. The dual space $\mathcal{FZ}^\vee$ is thus the subspace of $\mathbb{Q}\langle x, y\rangle$ that annihilates the elements of $\mathcal{I}_{\mathcal{FZ}}$; explicitly,

$\mathcal{FZ}^\vee \subset \mathbb{Q}\langle x, y\rangle$ is a weight-graded space in which $\mathcal{FZ}_0^\vee = \mathbb{Q}$, $\mathcal{FZ}_1^\vee = 0$ and for $w \geq 2$, $\mathcal{FZ}_w^\vee$ consists of all degree w homogeneous polynomials $P \in \mathbb{Q}\langle x, y\rangle$ satisfying

$$\langle L, P\rangle = 0 \quad \text{for all } L \in \mathcal{I}_{\mathcal{FZ}}\,, \tag{3.2}$$

for the pairing in (3.1) (see Definition 2.1.1 for an explicit description of the elements L of the ideal $\mathcal{I}_{\mathcal{FZ}}$). The subspace $\mathcal{F}^\vee$ is strictly smaller than $\mathbb{Q}\langle x, y\rangle$. In weight $w = 2$, for instance, since $Z(xy) + Z(yx) \in \mathcal{I}_{\mathcal{FZ}}$, we have $xy - yx \in \mathcal{FZ}_2^\vee$ whereas xy and yx are not individually contained in $\mathcal{FZ}_2^\vee$.

Similarly, the dual space of the quotient $\overline{\mathcal{FZ}}$ of $\mathcal{FZ}$ modulo $\zeta_2^{\mathfrak{f}}$ is a subspace $\overline{\mathcal{FZ}}^\vee \subset \mathcal{FZ}^\vee$. We now consider $\overline{\mathcal{FZ}}$ with its Hopf algebra structure given by the coproduct Δ^G; then the dual space $\overline{\mathcal{FZ}}^\vee$ is also a Hopf algebra. The coproduct on $\overline{\mathcal{FZ}}^\vee$ is inherited directly from the standard coproduct Δ_s on $\mathbb{Q}\langle x, y\rangle$, given by

$$\Delta_s(x) = x \otimes \mathbf{1} + \mathbf{1} \otimes x\,, \qquad \Delta_s(y) = y \otimes \mathbf{1} + \mathbf{1} \otimes y\,; \tag{3.3}$$

it satisfies

$$\langle \xi_1 \otimes \xi_2, \Delta_s(g)\rangle = \langle \xi_1 ⧢ \xi_2, g\rangle \tag{3.4}$$

for $g \in \overline{\mathcal{FZ}}^\vee$, $\xi_1, \xi_2 \in \overline{\mathcal{FZ}}$. The multiplication on $\overline{\mathcal{FZ}}^\vee$, which we denote by $\diamond$, is uniquely determined by the equality

$$\langle \Delta^G(\xi), g \otimes h\rangle = \langle \xi, g \diamond h\rangle \tag{3.5}$$

for $\xi \in \overline{\mathcal{FZ}}$ and $g, h \in \overline{\mathcal{FZ}}^\vee$, and an explicit formula for $g \diamond h$ in the restricted case of $g \in \mathfrak{fz}^\vee$ can be found in (3.17) below.

Let us now explain how to view $\overline{\mathcal{FZ}}^\vee$ as the universal enveloping algebra of the Lie algebra consisting of its primitive elements. We begin by identifying the subspace $\mathrm{Lie}[x, y]$ of Lie polynomials in $\mathbb{Q}\langle x, y\rangle$ as the subspace of primitive elements, which are those satisfying

$$\Delta_s(g) = g \otimes \mathbf{1} + \mathbf{1} \otimes g\,. \tag{3.6}$$

An equivalent formulation of this property is that g is a Lie polynomial in $\mathbb{Q}\langle x, y\rangle$ if and only if

$$\langle Z(u ⧢ v)\,,\, g\rangle = 0\,, \tag{3.7}$$

for all pairs of non-empty words u, v. The Lie subalgebra of the Hopf algebra $\overline{\mathcal{FZ}}^\vee$ is likewise the space of elements $g \in \overline{\mathcal{FZ}}^\vee$ satisfying (3.6); the Lie bracket is given by

$$\{g, h\} \coloneqq g \diamond h - h \diamond g\,, \tag{3.8}$$

for the multiplication $\diamond$ of (3.5).

This Lie algebra is identified with the dual of the space $\mathfrak{fz}$ defined in (2.49) above; indeed, the vector space $\mathfrak{fz}$ inherits the structure of a Lie coalgebra from the Hopf algebra structure on $\overline{\mathcal{FZ}}$, so its dual space $\mathfrak{fz}^\vee \subset \overline{\mathcal{FZ}}^\vee$ thus forms a Lie algebra, which is precisely the Lie algebra of primitive elements of $\overline{\mathcal{FZ}}^\vee$.

Since $\mathfrak{fz}$ is the quotient of $\overline{\mathcal{FZ}}$ modulo non-trivial products and the relations

$$\begin{aligned} \zeta^{\mathfrak{f}}(u)\zeta^{\mathfrak{f}}(v) &= \zeta^{\mathfrak{f}}(u \sqcup\!\sqcup v)\,, \\ \zeta^{\mathfrak{f}}_*(u)\zeta^{\mathfrak{f}}_*(v) &= \zeta^{\mathfrak{f}}_*(u * v)\,, \end{aligned} \tag{3.9}$$

hold in $\mathcal{FZ}$ (the second equality being valid whenever u, v both end in y), we see that the images of $\zeta^{\mathfrak{f}}(w)$ in the quotient $\mathfrak{fz}$ satisfy

$$\zeta^{\mathfrak{f}}(u \sqcup\!\sqcup v) = \zeta^{\mathfrak{f}}_*(u * v) = 0 \quad \text{in } \mathfrak{fz}\,. \tag{3.10}$$

Thus the dual space $\mathfrak{fz}^\vee$ is the subspace of polynomials $g \in \mathbb{Q}\langle x, y\rangle$ such that

$$\langle Z(u \sqcup\!\sqcup v), g\rangle = \langle Z_*(u * v), g_*\rangle = 0\,, \tag{3.11}$$

for all pairs of monomials u and v (ending in y for the $*$ term), where

$$g_* = g + \sum_{n\geq 2} \frac{(-1)^{n-1}}{n} \zeta(x^{n-1}y)y^n\,, \tag{3.12}$$

(the term added to g is the linearized version of (2.10)). We note in particular that by (3.7), the first equality $\langle Z(u \sqcup\!\sqcup v), g\rangle = 0$ shows that we have an inclusion of vector spaces (which is not a Lie algebra morphism as the brackets are different)

$$\mathfrak{fz}^\vee \subset \mathrm{Lie}[x, y]\,. \tag{3.13}$$

The Lie algebra $\mathfrak{fz}^\vee$ is known as the *double shuffle Lie algebra* and usually denoted by $\mathfrak{ds}$ for "double shuffle" (or $\mathfrak{dmr}$ for "double mélange régularisé" by French authors). The Lie bracket $\{\cdot, \cdot\}$ on $\mathfrak{ds}$ corresponds to the Ihara bracket

$$\{g, h\} = [g, h] + D_g(h) - D_h(g)\,, \tag{3.14}$$

where for each $g \in \mathrm{Lie}[x, y]$, the *Ihara derivation* D_g of $\mathrm{Lie}[x, y]$ is defined by

$$D_g(x) = 0\,, \qquad D_g(y) = [y, g]\,, \tag{3.15}$$

and the Lie bracket arises from the bracket of derivations

$$[D_g, D_h] = D_{\{g,h\}}\,. \tag{3.16}$$

The Hopf algebra $\overline{\mathcal{FZ}}^\vee$ is identified with the universal enveloping algebra $\mathcal{U}\mathfrak{ds}$ (indeed, Goncharov originally developed his coproduct on $\overline{\mathcal{FZ}}$ by determining the Hopf algebra dual of $\mathcal{U}\mathfrak{ds}$). As such, the multiplication $\diamond$ is identified with the Poincaré–Birkhoff–Witt multiplication (which exists for every universal enveloping algebra of a Lie algebra).

Although the general expression of the $\diamond$ multiplication for two elements $g, h \in \mathcal{U}\mathfrak{ds}$ is complicated, in the case where $g \in \mathfrak{ds}$ and $h \in \mathcal{U}\mathfrak{ds}$ it simplifies to the rule

$$g \diamond h = gh + D_g(h)\,, \tag{3.17}$$

which suffices for our purposes and implies that the two representations (3.8) and (3.14) of the Ihara bracket agree.

In the rest of this article with the exception of section 4, we will consider the space $\mathcal{FZ}$ as a Hopf algebra comodule equipped with the coaction Δ^{GB} over the Hopf algebra $\overline{\mathcal{FZ}}$ equipped with the coproduct Δ^G; the multiplication $\diamond$ extends to $\mathcal{FZ}$ by the identity

$$\langle \Delta^{GB}(\xi), g \otimes h \rangle = \langle \xi, g \diamond h \rangle \tag{3.18}$$

for $\xi \in \mathcal{FZ}$ and $g, h \in \mathcal{MZ}^\vee$. The quotient space $\overline{\mathcal{MZ}}$ of $\overline{\mathcal{FZ}}$ is then also a Hopf algebra equipped with the coproduct Δ^G, and $\mathcal{MZ}$ equipped with Δ^{GB} is a Hopf algebra comodule over it. The dual space

$$\overline{\mathcal{MZ}}^\vee \subset \overline{\mathcal{FZ}}^\vee = \mathcal{U}\mathfrak{ds} \tag{3.19}$$

of $\overline{\mathcal{MZ}}$ is a Hopf algebra equipped with the standard coproduct Δ_s and the (restriction of the) multiplication $\diamond$, and the Lie algebra

$$\mathfrak{mz}^\vee \subset \mathfrak{fz}^\vee = \mathfrak{ds} \tag{3.20}$$

consists of the primitive elements for Δ_s in $\overline{\mathcal{MZ}}$, and is equipped with the (restriction of the) Ihara bracket (3.8).

3.2 The Z-map and dual spaces

Definition 3.2.1. We define the *Z-map* to be the canonical isomorphism

$$\mathbb{Q}\langle x, y\rangle \xrightarrow{Z} \mathbb{Q}[Z(w)] \tag{3.21}$$

mapping $\mathbf{1}$ to 1 and each non-trivial monomial w to $Z(w)$, so that the notation $Z(w)$, previously just a symbol (see section 2.1.2), can now be interpreted as the image of the monomial w under the map Z. The Z-map restricts to a canonical isomorphism on each (finite-dimensional) weight-graded part, and passes to corresponding isomorphisms (also called Z-maps) between any quotient of $\mathbb{Q}[Z(w)]$ (in particular the MZV spaces) and its dual viewed as a subspace of $\mathbb{Q}\langle x, y\rangle$.

The situation is summarized in (3.25) below, in which all of the horizontal arrows are the canonical isomorphisms inherited from the top Z-map

$$Z : \mathbb{Q}\langle x, y\rangle \to \mathbb{Q}[Z(w)]\,, \tag{3.22}$$

all surjective maps are quotients, and all injective maps are inclusions of the dual spaces. The space $\overline{\mathcal{Z}}$ denotes the quotient of the $\mathbb{Q}$-algebra $\mathcal{Z}$ of real MZVs modulo the ideal generated by ζ_2, and in analogy with $\mathfrak{fz}$ and $\mathfrak{mz}$, we denote the quotient of $\overline{\mathcal{Z}}$ mod constants and non-trivial products by $\mathfrak{z}$. For instance, the Z-map $Z(xy)$ is given by $\zeta_2^{\mathfrak{m}}$ in $\mathcal{MZ}$ and 0 in $\overline{\mathcal{MZ}}$, respectively. More generally, we have

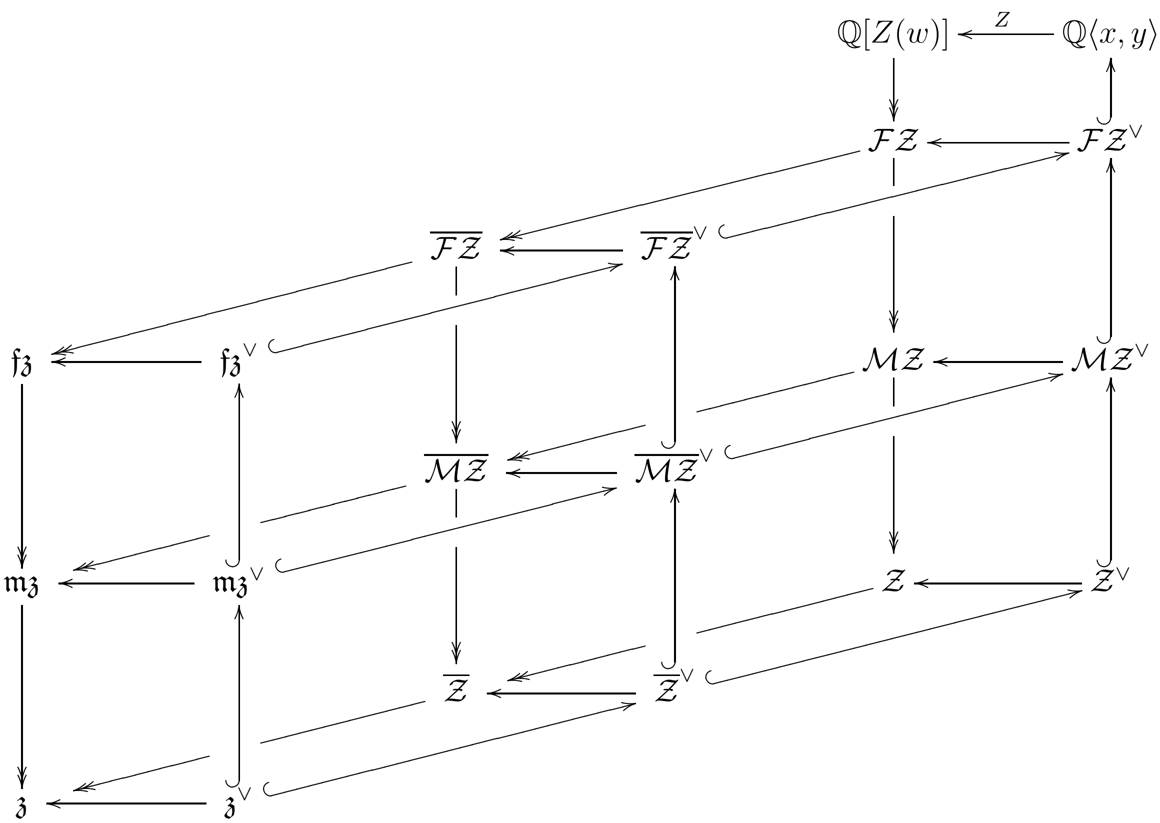
$$Z(x^{k_r-1}y\cdots x^{k_2-1}yx^{k_1-1}y) = \zeta^{\mathfrak{m}}_{k_1,k_2,\ldots,k_r} \text{ in } \mathcal{MZ} \tag{3.23}$$

for convergent words ($k_r \geq 2$), whereas the Z-map of divergent words follows from setting the combinations in (2.18) to zero.

Note that while both $\mathfrak{fz}$ and $\mathfrak{mz}$ are equipped with a Lie coalgebra structure inherited from the Hopf algebra structures on $\overline{\mathcal{FZ}}$ and $\overline{\mathcal{MZ}}$, we do not know that $\overline{\mathcal{Z}}$ is a Hopf algebra and therefore we do not know that $\mathfrak{z}$ has a Lie coalgebra structure. However we still have vector space surjections $\mathfrak{fz} \twoheadrightarrow \mathfrak{mz} \twoheadrightarrow \mathfrak{z}$ and the corresponding vector space inclusions of the dual spaces, all of which lie in the vector space Lie$[x, y]$ by (3.13):

$$\mathfrak{z}^\vee \subset \mathfrak{mz}^\vee \subset \mathfrak{fz}^\vee \subset \mathrm{Lie}[x, y]\,. \tag{3.24}$$

We underline once more that all maps in the following diagram are to be viewed as vector space morphisms.



(3.25)

We will make constant use of the Z-maps as well as the quotient maps and inclusions in this diagram for our constructions below.

3.3 The canonical decomposition of motivic MZV spaces and zeta generators in genus zero

In this section we will define a specific canonical decomposition of $\mathcal{MZ}_w$ for each weight $w \geq 2$ into singles, irreducibles and reducibles of the type

$$\mathcal{MZ}_w = \mathbb{Q}\zeta_w^{\mathfrak{m}} \oplus I_w \oplus R_w \tag{3.26}$$

introduced in (2.54).

Definition 3.3.1. For each $w \geq 2$, let $\hat{R}_w \subset \mathcal{MZ}_w$ denote the subspace of reducible MZVs as in section 2.2.2, let $\mathfrak{mz}_w = \mathcal{MZ}_w/\hat{R}_w$ as in (2.52), let $\mathfrak{mz}_w^\vee \subset \mathcal{MZ}_w^\vee$ denote the dual space, and let $(\mathfrak{mz}_w^\vee)^{\geq 2} \subset \mathfrak{mz}_w^\vee$ denote the subspace of $\mathfrak{mz}_w^\vee$ consisting of elements of depth ≥ 2, where we recall that depth is the minimal y-degree of a polynomial.

- Define the *canonical subspace of non-single irreducibles* I_w of $\mathcal{MZ}_w$ by

$$I_w = Z\big((\mathfrak{mz}_w^\vee)^{\geq 2}\big) \subset \mathcal{MZ}_w\,. \tag{3.27}$$

- Define the *canonical subspace of non-single reducibles* R_w as follows. For odd weights w, set $R_w = \hat{R}_w$, and for even weights w, let $R_w \subset \hat{R}_w$ be the subspace spanned by all weight w products of the elements: $\zeta_2^{\mathfrak{m}}$, the single zetas $\zeta_v^{\mathfrak{m}}$ for odd $v < w$, and all elements of I_v with $v < w$, excluding only the product $(\zeta_2^{\mathfrak{m}})^{w/2}$. Then since $\mathcal{MZ} = \mathbb{Q}[\zeta_2^{\mathfrak{m}}] \otimes_{\mathbb{Q}} \overline{\mathcal{MZ}}$ (cf. (2.39)), using (2.51), we have $\hat{R}_w = \mathbb{Q}\zeta_w^{\mathfrak{m}} \oplus R_w$ when w is even.

- Define the *canonical decomposition* of $\mathcal{MZ}_w$ to be

$$\mathcal{MZ}_w = \mathbb{Q}\zeta_w^{\mathfrak{m}} \oplus I_w \oplus R_w \tag{3.28}$$

  for the canonical subspaces R_w and I_w defined above.

- Finally, define the *canonical polynomial* $g_w \in \mathcal{MZ}_w^\vee$ for each $w \geq 2$ to be the unique polynomial in x, y that

  – takes the value 1 on $\zeta_w^{\mathfrak{m}} = \zeta^{\mathfrak{m}}(x^{w-1}y)$ in the sense that $\langle Z(x^{w-1}y), g_w\rangle = 1$, and

  – annihilates I_w and R_w in the sense that $\langle \xi, g_w\rangle = 0$ for any $\xi \in I_w$ and $\xi \in R_w$.

Examples of the polynomials g_w will be given in section 3.4 below.

Lemma 3.3.2. *The canonical polynomials g_w for $w \geq 2$ are uniquely characterized by the following properties:*

(i) The polynomial g_w is normalized by $g_w|_{x^{w-1}y} = 1$;

(ii) The polynomial g_w lies in the subspace $(\mathcal{MZ}_w/R_w)^\vee \subset \mathcal{MZ}_w^\vee$; in particular for odd w it lies in $\mathfrak{mz}_w$ and is thus a Lie polynomial;

(iii) If we consider g_w as lying in $(\mathcal{MZ}_w/R_w)^\vee$, the image $Z(g_w)$ of g_w under the Z-map is a rational multiple of $\zeta^{\mathfrak{m}}_w \in \mathcal{MZ}_w/R_w$; equivalently, if we consider g_w as lying in $\mathcal{MZ}^\vee_w$, then

$$Z(g_w) \in \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus R_w \subset \mathcal{MZ}_w\,. \tag{3.29}$$

Proof. (i) is equivalent to $\langle Z(x^{w-1}y), g_w\rangle = 1$.

For (ii), saying that g_w annihilates R_w is equivalent to saying that g_w lies in the dual space of $\mathcal{MZ}_w/R_w$, namely $(\mathcal{MZ}_w/R_w)^\vee$; this space is equal to $\mathfrak{mz}^\vee_w$ when w is odd, so by (3.24) g_w is then in $\mathrm{Lie}[x, y]$.

For (iii), we consider $g_w \in (\mathcal{MZ}_w/R_w)^\vee$ and for $\mathcal{MZ}_w/R_w = \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus I_w$ we choose any basis consisting of $\zeta^{\mathfrak{m}}_w$ and a basis for I_w. Then since $\langle g_w, I_w\rangle = 0$ for all $\xi \in I_w$ we have $\langle Z(g_w), Z^{-1}(I_w)\rangle = 0$, but $Z^{-1}(I_w) = (\mathfrak{mz}^\vee_w)^{\geq 2}$, and the subspace of $\mathcal{MZ}_w/R_w$ annihilated by $(\mathfrak{mz}^\vee_w)^{\geq 2}$ is the 1-dimensional subspace generated by $\zeta^{\mathfrak{m}}_w$. Therefore if g_w is considered as lying in $(\mathcal{MZ}_w/R_w)^\vee$ we have $Z(g_w) \in \mathbb{Q}\zeta^{\mathfrak{m}}_w \subset \mathcal{MZ}_w/R_w$, or equivalently, if g_w is considered as lying in $\mathcal{MZ}_w$, we have $Z(g_w) \in \mathbb{Q}\zeta^{\mathfrak{m}}_w \oplus R_w$. □

Remark 3.3.3. The lemma shows that in order to compute the canonical polynomials g_w for any $w \geq 2$, once conditions (i) and (ii) of Lemma 3.3.2 are fulfilled, the third defining condition of g_w, namely that it annihilates the subspace I_w, can be replaced by condition (iii) of the Lemma, which does not require computing the space I_w. Once g_w is determined, it is then possible to recover the space I_w as the image under Z as in (3.27) if needed. However, we will provide a very natural explicit basis for I_w, called *the semi-canonical basis*, in section 3.5 below.

Definition 3.3.4. The set of g_w for odd $w \geq 3$ form a canonical generating set for $\mathfrak{mz}^\vee$, and their Ihara derivations (3.15) are referred to as *zeta generators in genus zero*. By Lemma 3.3.2, each g_w is characterized uniquely as the only depth 1 element of $\mathfrak{mz}_w$ normalized by $g_w|_{x^{w-1}y} = 1$ such that $Z(g_w)$ is a rational multiple of $\zeta^{\mathfrak{m}}_w \in \mathfrak{mz}$.

The method of using the Z-map to produce canonical generators by taking the duals of the single zetas was initially developed in the framework of formal multizetas in [17]. The family of polynomials g_w will play a crucial role in the main results of this paper, namely

- the construction of a canonical isomorphism $\rho : \mathcal{MZ} \to \mathcal{F}$ from the motivic MZVs to the f-alphabet (section 4.2);
- the construction of a canonical set of zeta generators in genus one (section 5.3).

In the next subsection we give the explicit calculation of the canonical decomposition in weights up to $w = 11$ and spell out the canonical polynomials g_w up to $w = 7$.

3.4 The canonical decomposition for $\mathcal{MZ}_w$ for $w \le 11$

Since all MZVs in this subsection and the next one are motivic, we drop the superscript $\mathfrak{m}$ and simply write $\zeta_{k_1,\dots,k_r}$ instead of $\zeta^{\mathfrak{m}}_{k_1,\dots,k_r}$. We have

$$
\begin{aligned}
\mathcal{MZ}_2 &= \langle \zeta_2 \rangle \,, \\
\mathcal{MZ}_3 &= \langle \zeta_3 \rangle \,, \\
\mathcal{MZ}_4 &= \langle \zeta_4 \rangle \,, \\
\mathcal{MZ}_5 &= \langle \zeta_5 \rangle \oplus \langle \zeta_2\zeta_3 \rangle = \mathbb{Q}\zeta_5 \oplus R_5 \,, \\
\mathcal{MZ}_6 &= \langle \zeta_6 \rangle \oplus \langle \zeta_3^2 \rangle = \mathbb{Q}\zeta_6 \oplus R_6 \,, \\
\mathcal{MZ}_7 &= \langle \zeta_7 \rangle \oplus \langle \zeta_2\zeta_5 \,,\ \zeta_2^2\zeta_3 \rangle = \mathbb{Q}\zeta_7 \oplus R_7 \,, \\
\mathcal{MZ}_8 &= \langle \zeta_8 \rangle \oplus \langle Z_{35} \rangle \oplus \langle \zeta_3\zeta_5 \,,\ \zeta_2\zeta_3^2 \rangle = \mathbb{Q}\zeta_8 \oplus I_8 \oplus R_8 \,, \\
\mathcal{MZ}_9 &= \langle \zeta_9 \rangle \oplus \langle \zeta_3^3 \,,\ \zeta_2\zeta_7 \,,\ \zeta_4\zeta_5 \,,\ \zeta_6\zeta_3 \rangle = \mathbb{Q}\zeta_9 \oplus R_9 \,, \\
\mathcal{MZ}_{10} &= \langle \zeta_{10} \rangle \oplus \langle Z_{37} \rangle \oplus \langle \zeta_3\zeta_7 \,,\ \zeta_5^2 \,,\ \zeta_2\zeta_3\zeta_5 \,,\ \zeta_2 Z_{35} \,,\ \zeta_4\zeta_3^2 \rangle = \mathbb{Q}\zeta_{10} \oplus I_{10} \oplus R_{10} \,, \\
\mathcal{MZ}_{11} &= \langle \zeta_{11} \rangle \oplus \langle Z_{335} \rangle \oplus \langle \zeta_3 Z_{35} \,,\ \zeta_3^2\zeta_5 \,,\ \zeta_2\zeta_9 \,,\ \zeta_2\zeta_3^3 \,,\ \zeta_4\zeta_7 \,,\ \zeta_6\zeta_5 \,,\ \zeta_8\zeta_3 \rangle = \mathbb{Q}\zeta_{11} \oplus I_{11} \oplus R_{11} \,,
\end{aligned}
\tag{3.30}
$$

where the irreducibles Z_{35}, Z_{37} and Z_{335} are the Z-map images of the generators $\{g_3, g_5\}$, $\{g_3, g_7\}$ and $\{g_3, \{g_3, g_5\}\}$ of $(\mathfrak{mz}_w^\vee)^{\ge 2}$ for $w = 8, 10$ and 11, respectively: they are explicitly given in terms of a common (arbitrary) choice of MZVs $\zeta_{3,5}$, $\zeta_{3,7}$ and $\zeta_{3,3,5}$ by

$$
\begin{aligned}
Z_{35} &:= Z(\{g_3, g_5\}) = -\tfrac{1105181}{80}\zeta_8 + \tfrac{24453}{5}\zeta_{3,5} + \tfrac{28743}{2}\zeta_3\zeta_5 - 1683\,\zeta_2\zeta_3^2 \,, \\
Z_{37} &:= Z(\{g_3, g_7\}) = \tfrac{6614309}{112}\zeta_{3,7} + \tfrac{7796217}{16}\zeta_3\zeta_7 + \tfrac{26525967}{112}\zeta_5^2 - \tfrac{2159}{627}\zeta_2 Z_{35} \\
&\qquad - \tfrac{3203187}{76}\zeta_2\zeta_3\zeta_5 - \tfrac{60072829}{608}\zeta_4\zeta_3^2 - \tfrac{408872741707}{680960}\zeta_{10} \,, \\
Z_{335} &:= Z(\{g_3, \{g_3, g_5\}\}) = -\tfrac{3683808}{5}\zeta_{3,3,5} + \tfrac{1119631493}{20}\zeta_{11} - \tfrac{28597725}{38}\zeta_3^2\zeta_5 \\
&\qquad + \tfrac{296304}{2717}\zeta_3 Z_{35} - \tfrac{198893689}{6}\zeta_2\zeta_9 + \tfrac{25828428}{247}\zeta_2\zeta_3^3 - \tfrac{90515817}{40}\zeta_4\zeta_7 \\
&\qquad + \tfrac{6826931}{4}\zeta_6\zeta_5 + \tfrac{1953356831}{23712}\zeta_8\zeta_3 \,.
\end{aligned}
\tag{3.31}
$$

We observe here that the products listed above spanning the spaces of reducibles R_w actually form bases for these spaces. This is a general result valid for all w, which will be proven in the following section 3.5, in which we actually determine an explicit basis for $\mathcal{MZ}$ adapted to the canonical decomposition of Definition 3.3.1.

Up to $w = 7$, the polynomials g_w are given by

$$
\begin{aligned}
g_2 &= [xy] \,, \\
g_3 &= [x[xy]] + [[xy]y] \,, \\
g_4 &= [x[x[xy]]] + \tfrac{1}{4}[x[[xy]y]] + [[[xy]y]y] + \tfrac{5}{4}(xyxy - xyyx - yxxy + yxyx) \,, \\
g_5 &= [x[x[x[xy]]]] + 2[x[x[[xy]y]]] - \tfrac{3}{2}[[x[xy]]\,[xy]] + 2[x[[[xy]y]y]] + \tfrac{1}{2}[[xy]\,[[xy]y]] + [[[[xy]y]y]y] \,,
\end{aligned}
$$

$$
\begin{aligned}
g_6 = {} & [x[x[x[x[xy]]]]]+\tfrac{3}{4}[x[x[x[[xy]y]]]]+\tfrac{1}{6}[x[[x[xy]]\,[xy]]]+\tfrac{23}{16}[x[x[[[xy]y]y]]]+\tfrac{1}{12}[x[[xy]\,[[xy]y]]] \\
& -\tfrac{89}{48}[x[[[xy]y]\,[xy]]]+\tfrac{3}{4}[x[[[[xy]y]y]y]]+\tfrac{5}{3}[[xy]\,[[[xy]y]y]]+[[[[[xy]y]y]y]y] \\
& +\tfrac{7}{4}(xyxxxy-xyyxxx+xyyyxy-xyyyyx-yxxxxy+yxyxxx-yyyxxy+yyyxyx) \\
& +\tfrac{21}{4}(xyxyxx-xyxxyx+yxxxyx-yxxyxx-yxyyxy+yxyyyx+yyxyxy-yyxyyx) \\
& +\tfrac{7}{16}(xyxxyy-xyyyxx-yxxxyy+yxyyxx)+\tfrac{7}{48}(yxxyxy-xyxyxy) \\
& +\tfrac{35}{48}(yxxyyx+yxyxxy-xyxyyx-xyyxxy)+\tfrac{77}{48}(xyyxyx-yxyxyx)\,, \\
g_7 = {} & [x[x[x[x[x[xy]]]]]]+3[x[x[x[x[[xy]y]]]]]-5[x[x[[x[x,y]]\,[x,y]]]]+2[[x[x[xy]]\,[x[xy]]] \\
& +5[x[x[x[[[xy]y]y]]]]+\tfrac{19}{16}[x[x[[xy]\,[[xy]y]]]]-\tfrac{173}{16}[x[[x[[xy]y]]\,[xy]]]-2[[x[xy]]\,[x[[xy]y]]] \\
& +\tfrac{17}{16}[[[x[xy]]\,[xy]]\,[xy]]+5[x[x[[[[xy]y]y]y]]]+\tfrac{99}{16}[x[[xy]\,[[[xy]y]y]]]-\tfrac{61}{16}[[x[[xy]y]]\,[[xy]y]] \\
& -\tfrac{109}{16}[[x[[[xy]y]y]]\,[xy]]+\tfrac{65}{16}[[xy]\,[[xy]\,[[xy]y]]]+3[x[[[[[xy]y]y]y]y]]+4[[xy]\,[[[[xy]y]y]y]] \\
& +3[[[xy]y]\,[[[xy]y]y]]+[[[[[[xy]y]y]y]y]y]\,.
\end{aligned}
\tag{3.32}
$$

In these expressions, we have omitted the separating comma between the two arguments of the Lie bracket in $\mathrm{Lie}[x,y]$ to condense the formulas. The odd degree (Lie) polynomials satisfy the symmetry property $g_{2k+1}(x,y)=g_{2k+1}(y,x)$ that follows from the arguments in footnote 11. This is easy to see for g_3, but requires also the use of the Jacobi identity to make it manifest for g_5 and g_7. Our expressions are chosen to be adapted to the Lyndon basis of $\mathrm{Lie}[x,y]$ that we introduce in the next section.

For $w\geq 8$ the polynomials g_w become too unwieldy to write down, although they can be calculated on a computer easily (either by the methods presented here, or from the Drinfeld associator as in (3.49) below). The explicit form of all g_w at $w\leq 12$ can be found in machine-readable form in an ancillary file of the arXiv submission of this work. However, since the Z-map is an isomorphism, no information is lost in giving their Z-map images, which determine them completely and are much shorter to write down:

$$
\begin{aligned}
Z(g_2) &= 2\zeta_2\,, \\
Z(g_3) &= 12\zeta_3\,, \\
Z(g_4) &= \tfrac{375}{8}\zeta_4\,, \\
Z(g_5) &= 385\zeta_5-105\zeta_2\zeta_3\,, \\
Z(g_6) &= \tfrac{251797}{288}\zeta_6-\tfrac{679}{4}\zeta_3^2\,, \\
Z(g_7) &= \tfrac{49203}{4}\zeta_7-\tfrac{14091}{4}\zeta_2\zeta_5-\tfrac{11865}{4}\zeta_4\zeta_3\,, \\
Z(g_8) &= \tfrac{769152355481}{40974336}\zeta_8-\tfrac{18246083}{1824}\zeta_3\zeta_5+\tfrac{74974943}{71136}\zeta_2\zeta_3^2\,, \\
Z(g_9) &= \tfrac{373659143}{864}\zeta_9-\tfrac{264398849}{3456}\zeta_6\zeta_3-\tfrac{3702413}{36}\zeta_4\zeta_5-\tfrac{70513729}{576}\zeta_2\zeta_7+\tfrac{133133}{16}\zeta_3^3\,, \\
Z(g_{10}) &= \tfrac{2256583872703076103276l}{48180785666457600}\zeta_{10}++\tfrac{23603271373}{184515876480}\zeta_2Z_{35}-\tfrac{70504768535925229}{227096463360}\zeta_3\zeta_7-\tfrac{66965094752611}{436723968}\zeta_5^2 \\
&\quad+\tfrac{21865877274704331}{321719989760}\zeta_2\zeta_3\zeta_5+\tfrac{3916397111572098571}{100376636805120}\zeta_4\zeta_3^2\,, \\
Z(g_{11}) &= \tfrac{1316030287522093}{78587904}\zeta_{11}+\tfrac{67235}{1227936}\zeta_3Z_{35}+\tfrac{4632642114815}{4911744}\zeta_3^2\zeta_5-\tfrac{824237896586533}{176822784}\zeta_2\zeta_9 \\
&\quad-\tfrac{470709526441}{4911744}\zeta_2\zeta_3^3-\tfrac{3026492983085}{818624}\zeta_4\zeta_7-\tfrac{218501860145855}{78587904}\zeta_6\zeta_5-\tfrac{3190686062952839}{1414582272}\zeta_8\zeta_3\,.
\end{aligned}
\tag{3.33}
$$

Note that, in agreement with the third characterizing property (3.29) of g_w, the non-single irreducibles $Z_{35}\in I_8$, $Z_{37}\in I_{10}$ and $Z_{335}\in I_{11}$ are absent in $Z(g_8)$, $Z(g_{10})$ and $Z(g_{11})$, respectively. The contributions $\zeta_2 Z_{35}$ and $\zeta_3 Z_{35}$ to $Z(g_{10})$ and $Z(g_{11})$ lie in R_{10} and R_{11}, respectively, and are therefore compatible with (3.29).

3.5 The semi-canonical basis for $\mathcal{MZ}_w$

In this section we determine an explicit basis for $\mathcal{MZ}$ which is adapted to the canonical decomposition. The basis of the irreducible parts I_w is given by the Z-map images of the Lyndon brackets of the canonical free generators g_w of $\mathfrak{mz}_w^\vee$. The basis of the reducible part R_w in turn consists of all weight w products of elements of the set given by ζ_2, ζ_v for all odd $v < w$, and the chosen basis elements for I_v for $v < w$, which form a linearly independent set as proven in Corollary 3.5.8 at the end of this subsection. Because the Lyndon basis for a free Lie algebra, although very natural and practical, cannot justifiably be called canonical, we refer to our basis as the *semi-canonical* basis for the canonical decomposition of $\mathcal{MZ}_w$.

Let us recall the definition and the basic result we need concerning Lyndon bases.

Definition 3.5.1. Let $B = \{b_1, b_2, \ldots\}$ be an ordered set of letters. A *Lyndon word* in the alphabet B is a word $W_1 = b_{i_1} b_{i_2} \cdots b_{i_r}$ that has the property that every right subword $W_j = b_{i_j} b_{i_{j+1}} \cdots b_{i_r}$ with $j > 1$ is lexicographically larger than W_1.

The following classic theorem was discovered simultaneously in 1958 by Chen–Fox–Lyndon and Shirshov (cf. [59], [60], or [61] for a comprehensive introduction).

Theorem 3.5.2. *Let $B = \{b_1, b_2, \ldots\}$ be an ordered set of letters and let* Lie$[B]$ *be the free Lie algebra generated by B (over a field which we take to be $\mathbb{Q}$). Then a basis of* Lie$[B]$ *is given by the individual letters b_i and the set of* Lyndon brackets

$$[b_{i_1} b_{i_2} \ldots b_{i_r}]\,, \tag{3.34}$$

where the word $b_{i_1} b_{i_2} \ldots b_{i_r}$ is a Lyndon word, and the rule for making it into a Lie bracket is to place the comma at the leftmost position such that it divides the Lyndon word into two shorter Lyndon words:

$$[b_{i_1} b_{i_2} \ldots b_{i_r}] = \big[[b_{i_1} \ldots b_{i_{k-1}}], [b_{i_k} \ldots b_{i_r}]\big] \tag{3.35}$$

and to proceed recursively until it is a multiple bracket of single letters for which we set $[b_i] \coloneqq b_i$.

Examples. The first few Lyndon brackets in the free Lie algebra Lie$[x, y]$ are given by

$$[xy] = [x, y]\,, \quad [xxy] = [x, [x, y]]\,, \quad [xyy] = [[x, y], y]\,, \quad [xxyy] = [x, [[x, y], y]]\,. \tag{3.36}$$

The first few Lyndon brackets in the free Lie algebra $\mathfrak{mz}^\vee$ on one generator g_w for each odd $w \geq 3$ (see Definition 3.3.4) equipped with its Ihara Lie bracket $\{\cdot, \cdot\}$ from (3.14) are given by

$$\{g_3 g_5\} = \{g_3, g_5\}\,, \quad \{g_3 g_7\} = \{g_3, g_7\}\,, \quad \{g_3 g_3 g_5\} = \{g_3, \{g_3, g_5\}\}\,. \tag{3.37}$$

Definition 3.5.3. Since $\mathfrak{mz}^\vee$ is freely generated by the canonical Lie polynomials $g_3, g_5, \ldots$, the Lyndon brackets in these generators form a basis. Every such Lyndon bracket corresponds as above to a Lyndon word $g_{v_1} \cdots g_{v_r}$ with $r > 1$. We write the corresponding Lyndon bracket as

$$L_{v_1 v_2 \cdots v_r} := \{g_{v_1} g_{v_2} \cdots g_{v_r}\} \in \mathfrak{mz}^\vee \,. \tag{3.38}$$

For example, L_{335} denotes the Lyndon bracket $\{g_3, \{g_3, g_5\}\}$. We denote the Z-map images of the Lyndon bracket by

$$Z_{v_1 \cdots v_r} := Z(L_{v_1 \cdots v_r}) \,, \tag{3.39}$$

consistently with (3.31). These elements with $v_1 + \cdots + v_r = w$ form the *semi-canonical basis* for the canonical subspace of weight w non-single irreducibles $I_w \subset \mathcal{MZ}_w$.

Our next task is to establish a basis for the spaces R_w.

Proposition 3.5.4. *Let $C_w \subset \mathcal{MZ}$ be the set consisting of ζ_2, the ζ_v for odd $3 \leq v < w$, and the Z-map images $Z_{v_1 \cdots v_r}$ of Lyndon brackets $L_{v_1 \cdots v_r} \in \mathfrak{mz}^\vee$ with $r > 1$, $v_1 + \cdots + v_r < w$. Then, the set of weight w products of elements of C_w forms a linearly independent set. If w is odd (resp. even) all of these products (resp. all of these products except for $(\zeta_2)^{w/2}$) form a basis for R_w.*

This proposition follows from the general result on Hopf algebras given in the following theorem (see Corollary 3.5.8). It seems like this result should be well-known, however it appears to have only been written down in an unpublished note by Perrin and Viennot [62].

Theorem 3.5.5. *Let X denote an alphabet of weighted letters having the property that the number of letters in each weight is finite. Let $A^\vee$ denote the graded associative $\mathbb{Q}$-algebra on X, considered as a Hopf algebra equipped with a multiplication denoted $\diamond$ and the standard coproduct Δ_s for which the letters of X are primitive. Let A denote the graded dual space of $A^\vee$, let $L^\vee \subset A^\vee$ denote the subspace of primitive elements for Δ_s, and let $B = \{b_1, b_2, \ldots\}$ be a vector space basis for $L^\vee$. Then,*

- *(i) $L^\vee$ forms a Lie algebra whose bracket is given by $[g, h] = g \diamond h - h \diamond g$.*
- *(ii) Both A and $A^\vee$ have bases given by the monomials w in the letters of X, which we denote by $w \in A$ and $w^\vee \in A^\vee$. The map $w^\vee \mapsto w$ provides an isomorphism of graded vector spaces from $A^\vee$ to A. As a $\mathbb{Q}$-algebra, however, A is commutative, equipped with the shuffle multiplication.*
- *(iii) Let ξ_i denote the images of the elements $b_i \in A^\vee$ under the isomorphism in (ii). The ξ_i then form a multiplicative set of generators for A under the shuffle multiplication.*
- *(iv) The ordered monomials $\xi_{i_1} ⧢ \xi_{i_2} ⧢ \cdots ⧢ \xi_{i_m}$ form a linear basis for A; those with $m > 1$ form a basis for the subspace $S \subset A$ annihilating $L^\vee$.*

Proof. (i) follows directly from the Milnor–Moore theorem [63]. The vector space part of (ii) follows from the fact that each graded part is finite-dimensional, so has a dual that is isomorphic to it and equipped with a dual basis; the notation $w^\vee$ for the basis of $A^\vee$ simply defines a dual basis to the basis of monomials $w \in A$. The fact that the multiplication on A is the shuffle is standard, corresponding to the fact that an element of $A^\vee$ is a Lie element if and only if it satisfies the shuffle relations (see (3.7)), completing the proof of (ii). This is the same as saying that the subspace $S \subset A$ spanned by all shuffles of monomials is the subspace that annihilates the Lie algebra $L^\vee$. For this reason, the quotient space $L = A/S$ is the Lie coalgebra dual to $L^\vee$, and the linear isomorphism in (ii) induces a linear isomorphism between L and $L^\vee$. Hence, the $\xi_i \in A$ form a basis for a subspace $\tilde{L} \subset A$ isomorphic to L, restricted to which the quotient map $A \to A/S = L$ is an isomorphism. Thus we have $A = S \oplus \tilde{L}$, completing the proof of (iii).

The final point (iv) follows from the Poincaré–Birkhoff–Witt theorem [64], which states that the universal enveloping algebra of a Lie algebra is generated by the ordered monomials in elements of a basis, and the only relations come from relations in the Lie algebra. We consider $L = A/S$ as a Lie algebra with the trivial bracket, so that the only multiplicative relations between the generators ξ_i of L are given by the fact that they commute. By the Poincaré–Birkhoff–Witt theorem, the ordered monomials $\xi_{i_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup \xi_{i_m}$ with $m \geq 1$ then form a basis for the universal enveloping algebra A of L, and the monomials with $m > 1$ form a basis for the kernel of the map $A \to L$, so in fact they form a basis for S, proving (iv).□

Remark 3.5.6. Essentially what this proof expresses is that the usual basis of the free associative algebra $A^\vee$ on the alphabet X, given by the monomials in the letters of X, can be replaced by a different basis consisting of the basis b_i of Lie elements on the one hand, spanning the Lie algebra $L^\vee \subset A^\vee$, completed by the space $S^\vee$ spanned by shuffles of monomials on the other, so that $A^\vee = L^\vee \oplus S^\vee$. In the dual space A, this corresponds to an equivalent decomposition $A = L \oplus S$ where L is the subspace whose basis is the ξ_i and S is the subspace spanned by all non-trivial shuffles of the ξ_i, which are in fact linearly independent by (iv).

Corollary 3.5.7. *Let $A^\vee = \overline{\mathcal{MZ}}^\vee$, which by Brown's theorem [15] is freely generated by $g_3, g_5, \ldots$ under the $\diamond$ multiplication. Then the elements $Z(g_w)$ for odd $w \geq 3$ together with the shuffles*

$$Z(g_{w_1}) \sqcup\!\sqcup Z(g_{w_2}) \sqcup\!\sqcup \cdots \sqcup\!\sqcup Z(g_{w_r}) \quad \text{with} \quad w_1 \leq w_2 \leq \cdots \leq w_r \tag{3.40}$$

(called ordered *shuffle products) form a basis for $\overline{\mathcal{MZ}} = A$; in particular the shuffles are linearly independent.*

We now pass from $\overline{\mathcal{MZ}}$ to $\mathcal{MZ}$ by using the isomorphism (2.39).

Corollary 3.5.8. *Let $g_3, g_5, \ldots$ denote the canonical generators of $\mathfrak{mz}^\vee$. Then a basis for $\mathcal{MZ}$ is given by the following elements:*

(i) the single motivic zeta values ζ_w for $w \geq 2$;

(ii) the Z-map images $Z_{w_1 \cdots w_r}$ of the basis of $\mathfrak{mz}^\vee$ given by the Lyndon brackets $L_{w_1 \cdots w_r}$ with $r > 1$ of the canonical generators $g_3, g_5, \ldots$; the weight $w = w_1 + \ldots + w_r$ elements of this type give a basis of I_w;

(iii) the ordered shuffle products of all the basis elements in (i) and (ii) above, excluding the products of even single zetas (since these products are equal to rational multiples of powers of ζ_2); the weight w elements of this type form a basis for R_w.

Proof. A basis of $\mathbb{Q}[\zeta_2]$ is given by the powers of ζ_2, so by (2.51) the single zeta values ζ_w for all even $w \geq 2$ also give a basis. A basis for $\overline{\mathcal{MZ}}$ is given in Corollary 3.5.7. Thanks to (2.39), a basis for the tensor product is given by the products of the basis elements of each of the two vector spaces, which is precisely as described by (i), (ii) and (iii) of the statement.□

3.6 Canonical polynomials from the Drinfeld associator

In this section we introduce the Drinfeld associator [18,19] which offers an alternative method of computing the canonical polynomials g_w. The Drinfeld associator is given by the power series [65]

$$\Phi_{\mathrm{KZ}}(x, y) \coloneqq \mathbf{1} + \sum_w (-1)^{d(w)} \zeta(w) w \in \mathcal{Z} \otimes_{\mathbb{Q}} \mathbb{Q}\langle\langle x, y \rangle\rangle \,, \tag{3.41}$$

where $\mathbb{Q}\langle\langle x, y\rangle\rangle$ denotes the degree completion of the polynomial ring $\mathbb{Q}\langle x, y\rangle$, the sum runs over non-trivial monomials w in x and y, and for each such w, $d(w)$ denotes the depth of the monomial, i.e. the number of y's contained in it.[5] Removing the signs in front of each term produces a power series that we call the *modified Drinfeld associator*, given by[6]

$$\Phi(x, y) \coloneqq \Phi_{\mathrm{KZ}}(x, -y) = \mathbf{1} + \sum_w \zeta(w) w \in \mathcal{Z} \,\hat{\otimes}\, \mathcal{Z}^\vee \,, \tag{3.42}$$

where $\hat{\otimes}$ denotes the completed tensor product (allowing infinite sums). We also have formal and motivic versions

$$\Phi^{\mathfrak{f}} \in \mathcal{FZ} \,\hat{\otimes}\, \mathcal{FZ}^\vee \quad \text{and} \quad \Phi^{\mathfrak{m}} \in \mathcal{MZ} \,\hat{\otimes}\, \mathcal{MZ}^\vee \,, \tag{3.43}$$

obtained by replacing $\zeta(w)$ by $\zeta^{\mathfrak{f}}(w)$ and $\zeta^{\mathfrak{m}}(w)$, respectively. The coefficients of all three power series Φ, $\Phi^{\mathfrak{f}}$ and $\Phi^{\mathfrak{m}}$ satisfy the regularized double shuffle relations.

[5] The subscript "KZ" in $\Phi_{\mathrm{KZ}}(x, y)$ stems from the fact that the Drinfeld associator can be constructed by solving the Knizhnik–Zamolodchikov equation, see appendix A.

[6] This definition gives an a posteriori explanation of the stuffle-regularized MZVs defined in (2.12): for words w ending with y the value $\zeta_*(w)$ is nothing other than the coefficient of w in the product $C\Phi$ of formal power series, where C is the power series defined in (2.10).

Definition 3.6.1. Let $V = \bigoplus_w V_w$ be a graded vector space for which each graded part is finite-dimensional, and let $V^\vee$ denote the graded dual (the direct sum of the duals of the graded parts of V). Choose any basis $e_1, e_2, \dots$ for V respecting the grading decomposition, and let $e_1^\vee, e_2^\vee, \dots$ denote the dual basis of $V^\vee$, with $\langle e_i^\vee, e_j \rangle = \delta_{ij}$. Let

$$\Psi = \sum_{i=1}^{\infty} e_i \otimes e_i^\vee \in V \mathbin{\hat{\otimes}} V^\vee . \tag{3.44}$$

We call Ψ the *canonical element* of $V \mathbin{\hat{\otimes}} V^\vee$.

Note that the element Ψ is independent of the choice of basis of V due to the use of dual bases.

Proposition 3.6.2. *Let V be as in Definition 3.6.1 and let $\phi : V \to W$ denote any surjective linear morphism and $\phi^\vee : W^\vee \to V^\vee$ denote the dual morphism. Let Ψ be the canonical element of $V \mathbin{\hat{\otimes}} V^\vee$. Then $\big(\phi \otimes (\phi^\vee)^{-1}\big)(\Psi)$ (in the sense specified in the proof) is the canonical element of $W \mathbin{\hat{\otimes}} W^\vee$.*

Proof. We may assume that V is finite-dimensional by working with a fixed graded piece. Since ϕ is surjective, we have that $V/\operatorname{Ker}\phi \cong W$. Choose a basis of V adapted to this quotient, i.e. linearly independent elements $\tilde{w}_1, \dots, \tilde{w}_m \in V$ that get mapped to a basis $\{w_i = \phi(\tilde{w}_i)\}$ of W under ϕ and a basis $k_1, \dots, k_n$ of $\operatorname{Ker}\phi$. Write the canonical element Ψ in this basis:

$$\Psi = \sum_{i=1}^{m} \tilde{w}_i \otimes \tilde{w}_i^\vee + \sum_{j=1}^{n} k_j \otimes k_j^\vee . \tag{3.45}$$

We now apply the map $\phi \otimes (\phi^\vee)^{-1}$ to Ψ, with the understanding that this map is interpreted as the composition

$$\big(\mathrm{id} \otimes (\phi^\vee)^{-1}\big) \circ (\phi \otimes \mathrm{id}) , \tag{3.46}$$

which avoids appearing to apply $(\phi^\vee)^{-1}$ to elements not in $\phi^\vee(W^\vee)$. We thus obtain

$$\big(\phi \otimes (\phi^\vee)^{-1}\big)(\Psi) = \sum_{i=1}^{m} w_i \otimes (\phi^\vee)^{-1}(\tilde{w}_i^\vee) = \sum_{i=1}^{m} w_i \otimes w_i^\vee , \tag{3.47}$$

which is the canonical element of $W \otimes W^\vee$. □

Recall from diagram (3.25) that $\mathbb{Q}[Z(w)]$ is the graded dual of the power series ring $\mathbb{Q}\langle\langle x, y \rangle\rangle$. Then, the element

$$\Phi^Z = \mathbf{1} + \sum_w Z(w) \otimes w \in \mathbb{Q}[Z(w)] \mathbin{\hat{\otimes}_{\mathbb{Q}}} \mathbb{Q}\langle\langle x, y \rangle\rangle \tag{3.48}$$

is the canonical element of the tensor product $\mathbb{Q}[Z(w)] \mathbin{\hat{\otimes}_{\mathbb{Q}}} \mathbb{Q}\langle\langle x, y \rangle\rangle$. Since $\mathcal{Z}, \mathcal{FZ}$ and $\mathcal{MZ}$, are all quotients of $\mathbb{Q}[Z(w)]$ (see diagram (3.25)), Proposition 3.6.2 then implies that Φ,

$\Phi^{\mathfrak{f}}$ and $\Phi^{\mathfrak{m}}$ are the canonical elements for the respective rings $\mathcal{Z}\,\hat{\otimes}\,\mathcal{Z}^\vee$, $\mathcal{FZ}\,\hat{\otimes}\,\mathcal{FZ}^\vee$ and $\mathcal{MZ}\,\hat{\otimes}\,\mathcal{MZ}^\vee$. In particular, the choice of basis in which to express $\Phi^{\mathfrak{m}}$ is of little significance in general. However, writing $\Phi^{\mathfrak{m}}$ in the semi-canonical basis does have one convenient advantage: it provides another method to compute the canonical polynomials g_w.

In our semi-canonical basis of $\mathcal{MZ}$ (see (3.31) for Z_{35}, Z_{37} and Z_{335}), the expansion of the modified Drinfeld associator Φ to weight 11 reads as follows, see [52] for the analogous expansion of the Drinfeld associator and its significance for the motivic coaction:[7]

$$
\begin{aligned}
\Phi = \mathbf{1} &+ \zeta_2 g_2 + \zeta_3 g_3 + \zeta_4 g_4 + \zeta_5 g_5 + \zeta_2\zeta_3 g_3 \diamond g_2 + \zeta_6 g_6 + \tfrac{1}{2}\zeta_3^2 g_3 \diamond g_3 + \zeta_7 g_7 \\
&+ \zeta_3\zeta_4 g_3 \diamond g_4 + \zeta_2\zeta_5 g_5 \diamond g_2 + \zeta_8 g_8 + \zeta_2\zeta_3^2\big(\tfrac{1}{2} g_3 \diamond g_3 \diamond g_2 + \tfrac{17}{247}\{g_3, g_5\}\big) \\
&+ \tfrac{1}{24453} Z_{35}\{g_3, g_5\} + \zeta_3\zeta_5\Big(\tfrac{47}{114} g_3 \diamond g_5 + \tfrac{67}{114} g_5 \diamond g_3\Big) \\
&+ \zeta_9 g_9 + \tfrac{1}{6}\zeta_3^3 g_3 \diamond g_3 \diamond g_3 + \zeta_2\zeta_7 g_7 \diamond g_2 + \zeta_4\zeta_5 g_5 \diamond g_4 + \zeta_6\zeta_3 g_3 \diamond g_6 \\
&+ \zeta_{10} g_{10} + \tfrac{8}{6614309} Z_{37}\{g_3, g_7\} + \zeta_3\zeta_7\big(\tfrac{24581}{59858} g_3 \diamond g_7 + \tfrac{35277}{59858} g_7 \diamond g_3\big) \\
&+ \zeta_5^2\big(\tfrac{1}{2} g_5 \diamond g_5 - \tfrac{2160}{29929}\{g_3, g_7\}\big) + \zeta_2 Z_{35}\big(\tfrac{1016}{243951279}\{g_3, g_7\} + \tfrac{1}{24453}\{g_3, g_5\} \diamond g_2\big) \\
&+ \zeta_2\zeta_3\zeta_5\big(\tfrac{47}{114} g_3 \diamond g_5 \diamond g_2 + \tfrac{67}{114} g_5 \diamond g_3 \diamond g_2 + \tfrac{492798}{9667067}\{g_3, g_7\}\big) \\
&+ \zeta_4\zeta_3^2\big(\tfrac{85}{494}\{g_3, g_5\} \diamond g_2 + \tfrac{60072829}{502687484}\{g_3, g_7\} + \tfrac{1}{2} g_3 \diamond g_3 \diamond g_4\big) \\
&+ \zeta_{11} g_{11} + \tfrac{1}{3683808} Z_{335}\{g_3, \{g_3, g_5\}\} \\
&+ \zeta_3 Z_{35}\big(\tfrac{7063}{625556646} g_3 \diamond g_3 \diamond g_5 + \tfrac{5728}{312778323} g_3 \diamond g_5 \diamond g_3 - \tfrac{6173}{208518882} g_5 \diamond g_3 \diamond g_3\big) \\
&+ \zeta_3^2\zeta_5\big(\tfrac{5439455}{46661568} g_3 \diamond g_3 \diamond g_5 + \tfrac{4179377}{23330784} g_3 \diamond g_5 \diamond g_3 + \tfrac{3177525}{15553856} g_5 \diamond g_3 \diamond g_3\big) \\
&+ \zeta_2\zeta_9\big(-\tfrac{31943}{22102848}\{g_3, \{g_3, g_5\}\} + g_9 \diamond g_2\big) + \zeta_4\zeta_7\big(\tfrac{46765}{3274496}\{g_3, \{g_3, g_5\}\} + g_7 \diamond g_4\big) \\
&+ \zeta_2\zeta_3^3\big(\tfrac{3066359}{75825048} g_3 \diamond g_3 \diamond g_5 - \tfrac{456995}{37912524} g_3 \diamond g_5 \diamond g_3 - \tfrac{2152369}{75825048} g_5 \diamond g_3 \diamond g_3 + \tfrac{1}{6} g_3 \diamond g_3 \diamond g_3 \diamond g_2\big) \\
&+ \zeta_8\zeta_3\big(-\tfrac{1953356831}{87350455296}\{g_3, \{g_3, g_5\}\} + g_3 \diamond g_8\big) + \zeta_6\zeta_5\big(\tfrac{540685}{14735232}\{g_3, \{g_3, g_5\}\} + g_5 \diamond g_6\big) + \ldots
\end{aligned}
\tag{3.49}
$$

Computational remarks

(1) In computing this expression, we have written multiple $\diamond$-products without parentheses with the understanding that we can evaluate them as $g_{w_1} \diamond (g_{w_2} \diamond \cdots (g_{w_{r-1}} \diamond (g_{w_r} \diamond g_k)) \cdots)$ with w_i odd and k odd or even. In this way, the left factor of each $\diamond$ multiplication is a Lie polynomial, i.e. a g_w with w odd, which allows us to use the simplified expression (3.17) for the multiplication $\diamond$ in $\mathcal{MZ}^\vee$.

(2) This gives us three ways to recursively compute the g_w, of which we saw the first two earlier:

(i) from the properties in Lemma 3.3.2 that uniquely characterize the g_w,

[7] The product $\circ$ among $h \in \mathfrak{ds}$ and $g \in \mathcal{U}\mathfrak{ds}$ in [52] is related to the Poincaré–Birkhoff–Witt multiplication $\diamond$ in (3.17) via $\overleftarrow{g \circ h} = \overleftarrow{h} \diamond \overleftarrow{g}$, where $\overleftarrow{w}$ is obtained by reversing the letters x, y of $w \in \mathbb{Q}\langle x, y\rangle$. This is a consequence of $D_{\overleftarrow{h}}(\overleftarrow{g}) = -\overleftarrow{D_h(g)}$ which can be proven by induction. The Drinfeld associator in the conventions of [52] is obtained from the series $\Phi(x, y)$ in the present work by reversing the words $w \mapsto \overleftarrow{w}$ in (3.42).

(ii) get the semi-canonical basis for I_w using the Lyndon words and then compute the unique normalized polynomial $g_w \in \mathcal{MZ}_w^\vee$ annihilating the basis elements of R_w and I_w, or

(iii) decompose Φ into the semi-canonical basis of $\mathcal{MZ}$; then

$$g_w = \Phi|_{\zeta_w} \tag{3.50}$$

The equivalence of the third approach with the others is a direct consequence of Proposition 3.6.2, which implies that the polynomial appearing in Φ with coefficient ζ_w must be the element of the dual basis of the semi-canonical basis taking the value 1 on ζ_w and annihilating I_w and R_w.

(3) As an advantage of the first method (i) over methods (ii) and (iii), the conditions of Lemma 3.3.2 make it clear that the canonical g_w do not depend on any basis choice for $\mathcal{MZ}_w$. For those weights w where the expansion of the Drinfeld associator is available (e.g. from [66, 67]), the third approach (iii) enjoys the computational advantage that ansätze and solutions of linear equation systems can be bypassed.

As pointed out earlier, in order to write motivic MZVs in a given basis in weight w we need to know the linear relations between motivic MZVs in that weight. While these are not known in general, we have several possible approaches: (i) in weights up to $w = 22$ (and also at weight $w = 23$ modulo a 31-bit prime), it is known by dimension arguments that $\mathcal{MZ}_w = \mathcal{FZ}_w$ [66] so we can use the double shuffle relations, (ii) since Brown gave the dimension of $\mathcal{MZ}_w$ in all weights, if we reached any weight where $\mathcal{MZ}_w$ is not equal to $\mathcal{FZ}_w$ (in spite of the conjecture that they are equal) we could write the real MZVs as real numbers, seek for enough linear relations between them with rational coefficients to reach the correct dimension and then prove that these relations are motivic [66]. In practice, the latter method has been used to create the available datamines, making the decomposition particularly easy by computer as it is enough to enter an MZV into the datamine to automatically obtain its decomposition. Note that the $\mathbb{Q}$-bases of [66] were extended from weight 22 to weight 34 in the HyperlogProcedures of Schnetz [67].

4 The canonical morphism from motivic MZVs to the f-alphabet

In [14, 15], Brown proved a remarkable theorem showing that the motivic MZV Hopf algebra comodule $\mathcal{MZ}$ is isomorphic to a certain Hopf algebra comodule $\mathcal{F}$ with a particularly simple structure that we recall below. However, Brown did not display a canonical isomorphism, but rather showed the existence and described the construction of a family of isomorphisms $\rho_{\vec{c}} : \mathcal{MZ} \to \mathcal{F}$ parametrized by free rational parameters $\vec{c}$ associated to a chosen basis of non-single irreducible motivic MZVs. The goal of this section is to use the canonical polynomials g_w of Definition 3.3.1 to fix a canonical choice of isomorphism

$$\rho : \mathcal{MZ} \to \mathcal{F} \,. \tag{4.1}$$

As in section 3.4, we will allow ourselves to simplify the notation by writing ζ instead of $\zeta^{\mathfrak{m}}$ throughout the present section, which will deal uniquely with motivic MZVs. Furthermore, in order for this section to remain coherent with the literature (see footnote 3 above) we will consider $\mathcal{MZ}$ as a Hopf algebra comodule with the structure conferred on it by the choice of coaction Δ_{GB} and not Δ^{GB} (see (2.31) and (2.36)). This change also modifies the structure of the dual Hopf algebra $\mathcal{MZ}^\vee$, which instead of being equipped with the multiplication $\diamond$ satisfying (3.18), becomes equipped with the multiplication $\bullet$ defined by

$$h \bullet g \coloneqq g \diamond h\,, \tag{4.2}$$

satisfying

$$\langle \Delta_{GB}(\xi), g \otimes h\rangle = \langle \xi, g \bullet h\rangle \tag{4.3}$$

for all $\xi \in \mathcal{MZ}$, $g, h \in \mathcal{MZ}^\vee$. Moreover, the simple expression (3.17) for $g \diamond h$ in case of $g \in \mathfrak{ds}$ translates into

$$h \bullet g = gh + D_g(h) \tag{4.4}$$

with the Ihara derivation D_g defined by (3.14). The Lie subspace of $\mathcal{MZ}^\vee$ is then equipped with the Lie bracket associated to $\bullet$, defined by

$$[\![g, h]\!] \coloneqq g \bullet h - h \bullet g\,. \tag{4.5}$$

(Note that this Lie bracket satisfies $[\![g, h]\!] = -\{g, h\}$ in relation to the Ihara bracket (3.14).)

4.1 Definition of the f-alphabet

We begin by defining the Hopf algebra comodule $\mathcal{F}$, familiarly called the f-alphabet [14,15]. To start with, let $\overline{\mathcal{F}}^\vee \coloneqq \mathbb{Q}\langle f_3^\vee, f_5^\vee, \ldots\rangle$ be the free associative Hopf algebra on one non-commutative indeterminate $f_w^\vee$ in each odd weight $w \geq 3$, with the usual (concatenation) multiplication and the standard coproduct defined by

$$\Delta_s(f_w^\vee) = f_w^\vee \otimes 1 + 1 \otimes f_w^\vee \tag{4.6}$$

for all odd $w \geq 3$. The subspace of Lie polynomials $\mathcal{L}^\vee \coloneqq \mathrm{Lie}[f_3^\vee, f_5^\vee, \ldots] \subset \overline{\mathcal{F}}^\vee$ is the space of primitive elements $f^\vee \in \overline{\mathcal{F}}^\vee$, i.e. elements satisfying

$$\Delta_s(f^\vee) = f^\vee \otimes 1 + 1 \otimes f^\vee\,. \tag{4.7}$$

Now let $\overline{\mathcal{F}}$ denote the Hopf algebra dual to $\overline{\mathcal{F}}^\vee$. The underlying vector space of $\overline{\mathcal{F}}$ is isomorphic to that of $\mathbb{Q}\langle f_3, f_5, \ldots\rangle$, the free associative algebra spanned by all monomials $f_{i_1}\cdots f_{i_r}$ in the free non-commutative indeterminates f_i for odd $i \geq 3$; these monomials form a dual basis to the basis of monomials $f_{i_1}^\vee \cdots f_{i_r}^\vee$ of $\overline{\mathcal{F}}^\vee$ in the sense that $\langle f_{i_1}^\vee \cdots f_{i_r}^\vee, f_{j_1}\cdots f_{j_r}\rangle = \delta_{i_1,j_1}\cdots\delta_{i_r,j_r}$. The Hopf algebra structure of $\overline{\mathcal{F}}$ is given by equipping $\overline{\mathcal{F}}$ with the (commutative) shuffle multiplication on the monomials $f_{i_1}\cdots f_{i_r}$ and the *deconcatenation coproduct* Δ defined by

$$\Delta(f_{i_1}\cdots f_{i_r}) = \sum_{j=0}^{r} f_{i_1}\cdots f_{i_j} \otimes f_{i_{j+1}}\cdots f_{i_r}\,. \tag{4.8}$$

Following Brown, let us now define the comodule $\mathcal{F}$ to be the tensor product

$$\mathcal{F} \coloneqq \mathbb{Q}[f_2] \otimes_{\mathbb{Q}} \overline{\mathcal{F}}\,, \tag{4.9}$$

where f_2 is a new commutative indeterminate of weight 2 and the factor $\mathbb{Q}[f_2]$ denotes the polynomial ring over $\mathbb{Q}$ in the single indeterminate f_2. The algebra structure of $\overline{\mathcal{F}}$ extends to $\mathcal{F}$ by letting f_2 commute with $\overline{\mathcal{F}}$; the general rule is

$$(f_2^m f_{i_1} \cdots f_{i_r}) ⧢ (f_2^n f_{j_1} \cdots f_{j_s}) = f_2^{m+n}\big(f_{i_1} \cdots f_{i_r} ⧢ f_{j_1} \cdots f_{j_s}\big) \tag{4.10}$$

for odd $i_1, \dots, i_r, j_1, \dots, j_s \geq 3$. By a slight abuse of terminology, we continue to call this product on all of $\mathcal{F}$ the *shuffle product* on $\mathcal{F}$.

The $\mathbb{Q}$-algebra $\mathcal{F}$ is made into a $\overline{\mathcal{F}}$-comodule by defining a coaction

$$\Delta : \mathcal{F} \to \mathcal{F} \otimes \overline{\mathcal{F}} \tag{4.11}$$

on $\mathcal{F}$ by (4.8) above together with

$$\Delta(f_2) = f_2 \otimes 1\,. \tag{4.12}$$

Thus the general formula for this coaction is given by

$$\Delta(f_2^n f_{i_1} f_{i_2} \dots f_{i_r}) = \sum_{j=0}^{r} f_2^n f_{i_1} \dots f_{i_j} \otimes f_{i_{j+1}} \dots f_{i_r} \tag{4.13}$$

with integer $n, r \geq 0$ and odd $i_j \geq 3$.

Now let $\mathcal{F}^\vee$ denote the dual of $\mathcal{F}$. The underlying vector space of $\mathcal{F}^\vee$ is a tensor product of two vector spaces

$$\langle f_2^\vee, f_4^\vee, \dots \rangle \otimes_{\mathbb{Q}} \overline{\mathcal{F}}^\vee\,, \tag{4.14}$$

where $\overline{\mathcal{F}}^\vee$ is as defined at the beginning of this section, and the left-hand factor denotes the vector space (not ring) dual of $\mathbb{Q}[f_2]$, with basis $f_{2n}^\vee \in \mathcal{F}^\vee$ satisfying

$$\langle f_{2n}^\vee, f_2^m \rangle = \delta_{m,n} \frac{\zeta_2^n}{\zeta_{2n}}\,. \tag{4.15}$$

By analogy with Definition 2.2.2 we set

$$f_{2m} \coloneqq \frac{\zeta_{2m}}{\zeta_2^m} f_2^m \in \mathcal{F}\,, \tag{4.16}$$

so that

$$\langle f_{2m}^\vee, f_{2n} \rangle = \delta_{m,n}\,. \tag{4.17}$$

The fact that $\mathcal{F}$ is a Hopf algebra comodule and not a Hopf algebra is reflected in the dual space by the fact that $\mathcal{F}^\vee$ is not a Hopf algebra but a Hopf algebra module over the Hopf algebra $\overline{\mathcal{F}}^\vee$. Thus, the concatenation multiplication does not extend from the subspace $\overline{\mathcal{F}}^\vee$ to all of $\mathcal{F}^\vee$; instead we only have an action of $\overline{\mathcal{F}}^\vee$ on $\mathcal{F}^\vee$, which we write as

$$a(f_{2n}^\vee b) = f_{2n}^\vee ab \in \mathcal{F}^\vee \tag{4.18}$$

for $n \geq 1$ and $a, b \in \overline{\mathcal{F}}^\vee$. This action can be considered as a multiplication of an element of the space $\mathbb{Q}[f_2^\vee, f_4^\vee, \ldots]$ with an element of $\overline{\mathcal{F}}^\vee$, but the $f_{2n}^\vee$ cannot be multiplied together. Thus every element of $\mathcal{F}^\vee$ is a sum of monomials which can be written uniquely in the form $f_{2n}^\vee b$ for some $n \geq 0$ (with the convention $f_0^\vee = 1$) and some $b \in \overline{\mathcal{F}}^\vee$.

4.2 A canonical choice of normalized isomorphism from $\mathcal{MZ}$ to $\mathcal{F}$

Definition 4.2.1. A morphism $\phi : \mathcal{MZ} \to \mathcal{F}$ is a *normalized morphism* if the following conditions hold [14, 15]:

(i) normalization: $\phi\big(\zeta_n\big) = f_n$ for all $n \geq 2$, where f_n for even values $n = 2m$ was defined in (4.16).

(ii) compatibility with the shuffle multiplication (4.10) on $\mathcal{F}$,

$$\phi\big(\zeta(w_1)\zeta(w_2)\big) = \phi\big(\zeta(w_1)\big) \sqcup \phi\big(\zeta(w_2)\big)\,. \tag{4.19}$$

(iii) compatibility with coactions Δ in (4.13) and Δ_{GB} in (2.42), given by the following formula for all monomials w in x and y:

$$\Delta\phi\big(\zeta(w)\big) = \phi\big(\Delta_{GB}\zeta(w)\big)\,. \tag{4.20}$$

It is understood that ϕ acts on each factor of the tensor product, with an additional projection from $\mathcal{F}$ to $\overline{\mathcal{F}}$ in the second factor, meaning that each term involving a power of f_2 in the second factor will be projected to zero.

Remark 4.2.2. The third property (4.20) translates the Goncharov–Brown coaction Δ_{GB}, which is expressed by the complicated procedure given in Definition 2.1.4, into the considerably simpler deconcatenation coaction (4.13) in the f-alphabet.

The results summarized in the next theorem follow directly from the results of Brown in [14, 15] that we state here in a version adapted to the semi-canonical basis of Definition 3.5.3.

Theorem 4.2.3 (Brown)**.** *Let $w \geq 2$, let $\mathcal{MZ}_w = \mathbb{Q}\zeta_w \oplus I_w \oplus R_w$ be the canonical decomposition of Definition 3.3.1 and choose the semi-canonical basis of I_w expressed via Lyndon words $Z_{v_1 \ldots v_r}$ introduced in Definition 3.5.3. Let $\vec{c} = \{c_{v_1 \ldots v_r}\}$ denote an infinite family of rational parameters indexed by the same Lyndon words. Then for any choice of rational values for the parameters $\vec{c}$, there exists a normalized Hopf algebra comodule isomorphism*

$$\rho_{\vec{c}} : \mathcal{MZ} \to \mathcal{F}\,. \tag{4.21}$$

Furthermore, any normalized Hopf algebra comodule isomorphism in the sense of Definition 4.2.1 corresponds to a specific choice of rational values of the parameters in $\vec{c}$.

Remark 4.2.4. We have used our choice of semi-canonical basis to state Brown's theorem, but the result is in fact independent of the choice of basis and even of the choice of subspace I_w of non-single irreducibles. For any such choice of I_w equipped with any basis, we can use that basis to index a set of rational numbers $\vec{c}$ parametrizing the inequivalent normalized isomorphisms from $\mathcal{MZ}$ to the f-alphabet, with the same constructive proof as the one indicated below for our particular choice.

Essentially, the proof of this result comes down to actually constructing the isomorphisms $\mathcal{MZ} \to \mathcal{F}$ inductively weight by weight [14, 15]. We sketch the procedure here and work it out explicitly for small weights.

We saw in section 3.5 that for weights $w \leq 7$ we have $I_w = \{0\}$. Thus for these weights the theorem says that the normalized isomorphism is uniquely fixed up to $w \leq 7$; it is in fact determined solely by properties (i) and (ii) of Definition 4.2.1. For $w = 2, 3, 4$, we must have

$$\begin{aligned} \rho_{\vec{c}} : \mathcal{MZ}_w &\to \mathcal{F}_w \,, \\ \zeta_w &\mapsto f_w \,, \end{aligned} \tag{4.22}$$

since the weight spaces $\mathcal{MZ}_w$ are 1-dimensional for these values. For weight 5, $\mathcal{MZ}_5$ is 2-dimensional spanned by ζ_5 and $\zeta_2\zeta_3$, so by (i) and (ii) we have

$$\begin{aligned} \rho_{\vec{c}} : \mathcal{MZ}_5 &\to \mathcal{F}_5 \,, \\ \zeta_5 &\mapsto f_5 \,, \\ \zeta_2\zeta_3 &\mapsto f_2 f_3 \,. \end{aligned} \tag{4.23}$$

For weight 6, $\mathcal{MZ}_6$ is 2-dimensional spanned by $\zeta_6 = \frac{35}{8}\zeta_2^3$ and ζ_3^2, so all $\rho_{\vec{c}}$ are given by

$$\begin{aligned} \rho_{\vec{c}} : \mathcal{MZ}_6 &\to \mathcal{F}_6 \,, \\ \zeta_6 &\mapsto f_6 \,, \\ \zeta_3^2 &\mapsto f_3 \sqcup\!\sqcup f_3 = 2 f_3 f_3 \,. \end{aligned} \tag{4.24}$$

Finally, in weight 7, $\mathcal{MZ}_7$ is 3-dimensional, spanned by ζ_7, $\zeta_2\zeta_5$ and $\zeta_3\zeta_4$, so we have

$$\begin{aligned} \rho_{\vec{c}} : \mathcal{MZ}_7 &\to \mathcal{F}_7 \,, \\ \zeta_7 &\mapsto f_7 \,, \\ \zeta_2\zeta_5 &\mapsto f_2 f_5 \,, \\ \zeta_2^2\zeta_3 &\mapsto f_2^2 f_3 \,. \end{aligned} \tag{4.25}$$

Starting from weight $w = 8$, the presence of non-trivial spaces of non-single irreducibles $I_w \subset \mathcal{MZ}_w$ requires additional input from the coaction property (4.20) in (iii).

Example. Let us illustrate this for the case of weight $w = 8$, where we use the element Z_{35} defined in (3.31) appearing in our semi-canonical basis constructed in section 3.5. The image under $\rho_{\vec{c}}$ of this element is not fixed by (i) and (ii) alone, so we make the most general ansatz

$$\rho_{\vec{c}}(Z_{35}) = a_1 f_3 f_5 + a_2 f_5 f_3 + a_3 f_2 f_3 f_3 + c_{35} f_8 \tag{4.26}$$

with rational parameters a_i, c_{35} and then impose (iii). By combining (3.31) and (2.44) we find that

$$\Delta_{GB}(Z_{35}) = Z_{35} \otimes 1 + 1 \otimes Z_{35} - \tfrac{20163}{2}\zeta_3 \otimes \zeta_5 + \tfrac{28743}{2}\zeta_5 \otimes \zeta_3 - 3366\zeta_2\zeta_3 \otimes \zeta_3 \,, \tag{4.27}$$

whose $\rho_{\vec{c}}$-image is

$$\rho_{\vec{c}}\big(\Delta_{GB}(Z_{35})\big) = \rho_{\vec{c}}(Z_{35}) \otimes 1 + 1 \otimes \rho_{\vec{c}}(Z_{35}) - \tfrac{20163}{2} f_3 \otimes f_5 + \tfrac{28743}{2} f_5 \otimes f_3 - 3366 f_2 f_3 \otimes f_3 \,. \tag{4.28}$$

To impose (iii) we have to compare this with the deconcatenation coaction (4.13) applied to the ansatz (4.26), which is

$$\Delta\big(\rho_{\vec{c}}(Z_{35})\big) = \rho_{\vec{c}}(Z_{35}) \otimes 1 + 1 \otimes \rho_{\vec{c}}(Z_{35}) + a_1 f_3 \otimes f_5 + a_2 f_5 \otimes f_3 + a_3 f_2 f_3 \otimes f_3 \,. \tag{4.29}$$

Comparing coefficients fixes the parameters a_i but leaves c_{35} undetermined, so for (4.26) we obtain

$$\rho_{\vec{c}}(Z_{35}) = -\tfrac{20163}{2} f_3 f_5 + \tfrac{28743}{2} f_5 f_3 - 3366 f_2 f_3^2 + c_{35} f_8 \,. \tag{4.30}$$

This is the first appearance of a rational parameter of $\vec{c}$ from Theorem 4.2.3. Analogous free parameters appear as the coefficient of f_w in the image under $\rho_{\vec{c}}$ of each basis element of I_w. In the semi-canonical basis the parameter $c_{v_1 \ldots v_r}$ corresponds to the coefficient of $f_{v_1 + \ldots + v_r}$ in $\rho_{\vec{c}}(Z_{v_1 \ldots v_r})$.

Definition 4.2.5. For $w \geq 8$, let $\mathcal{MZ}_w = \mathbb{Q}\zeta_w \oplus I_w \oplus R_w$ denote the canonical decomposition constructed in section 3.3. Let $\rho_{\vec{c}}$ be the family of normalized Hopf algebra comodule isomorphisms established in the semi-canonical basis as in Theorem 4.2.3 such that its rational parameters $\vec{c} = \{c_{v_1 \ldots v_r}\}$ are indexed by Lyndon words. Then we define the *canonical f-alphabet isomorphism*

$$\rho : \mathcal{MZ} \to \mathcal{F} \quad \text{by} \quad \rho \coloneqq \rho_{\vec{0}} \,. \tag{4.31}$$

The definition of the canonical isomorphism implies immediately

$$\rho(Z_{v_1 \ldots v_r})|_{f_w} = 0 \tag{4.32}$$

for all $v_1 + \ldots + v_r = w \geq 8$ (with $r > 1$), which is an alternative unique characterization of ρ. This leads for instance to

$$\begin{aligned}
\rho(Z_{35}) &= -\tfrac{20163}{2} f_3 f_5 + \tfrac{28743}{2} f_5 f_3 - 3366 f_2 f_3 f_3 \,, \\
\rho(Z_{37}) &= -\tfrac{5432401}{16} f_3 f_7 + \tfrac{7796217}{16} f_7 f_3 + 119340 f_5 f_5 - \tfrac{2698111}{16} f_4 f_3 f_3 - \tfrac{29731}{4} f_2 f_3 f_5 \\
&\quad - \tfrac{366535}{4} f_2 f_5 f_3 \,, \\
\rho(Z_{335}) &= 1629441 f_5 f_3 f_3 - 1037295 f_3 f_5 f_3 - 20223 f_3 f_3 f_5 + \tfrac{31943}{6} f_2 f_9 - 473832 f_2 f_3 f_3 f_3 \\
&\quad - \tfrac{420885}{8} f_4 f_7 - \tfrac{540685}{4} f_6 f_5 + \tfrac{1953356831}{23712} f_8 f_3 \,.
\end{aligned} \tag{4.33}$$

Proposition 4.2.6. *The isomorphism ρ is uniquely characterized by the property:*

$$\rho(\xi)|_{f_w} = 0 \text{ for all } \xi \in I_w \, . \tag{4.34}$$

Equivalently, one can characterize ρ as the unique isomorphism $\mathcal{MZ} \to \mathcal{F}$ that preserves the property (3.50), i.e.

$$\rho(\Phi)|_{f_w} = g_w \, . \tag{4.35}$$

Proof. Since the $Z_{v_1 \ldots v_r}$ at $v_1 + \ldots + v_r = w$ with $r > 1$ form a basis of I_w, we also have from (4.32) for all $w \geq 2$ that $\rho(\xi)|_{f_w} = 0$ for any $\xi \in I_w$. Therefore, writing Φ in the semi-canonical basis, no irreducible MZV can contribute to the coefficient of f_w in $\rho(\Phi)$ and the property (3.50) is preserved.

Note that even though the semi-canonical basis appears when defining $\rho = \rho_{\vec{0}}$ in (4.31), ρ is characterized by the property (4.34) which refers only to the *canonical* subspace I_w and therefore ρ can be defined canonically in this way. □

Remark 4.2.7. We end this section with a brief observation about the specific MZVs $\zeta_{3,5}$, $\zeta_{3,7}$ and $\zeta_{3,3,5}$, that are widely used in the physics literature as a basis for a non-canonical choice of (1-dimensional) subspace of non-single irreducibles in $I_w \subset \mathcal{MZ}_w$ for $w = 8, 10, 11$. Using (3.31) and (4.33), the canonical parameter choice $c_{35} = c_{37} = c_{335} = 0$ translates into the f-alphabet images

$$\begin{aligned} \rho(\zeta_{3,5}) &= -5 f_3 f_5 + \tfrac{100471}{35568} f_8 \, , \\ \rho(\zeta_{3,7}) &= -14 f_3 f_7 - 6 f_5 f_5 + \tfrac{408872741707}{40214998720} f_{10} \, , \\ \rho(\zeta_{3,3,5}) &= -5 f_3 f_3 f_5 - 45 f_2 f_9 - \tfrac{6}{5} f_2^2 f_7 + \tfrac{4}{7} f_2^3 f_5 + \tfrac{1119631493}{14735232} f_{11} \end{aligned} \tag{4.36}$$

for these elements. The analogous ρ-images of all irreducible higher-depth motivic MZVs of weights ≤ 17 in the basis choice of [66] can be found in the ancillary files of [8].

5 Canonical zeta generators σ_w in genus one

In this section we show how the canonical polynomials g_w associated with zeta generators in genus zero as defined in section 3.3 induce canonical zeta generators σ_w in genus one. The construction also includes a canonical split of σ_w into an arithmetic and a geometric part.

5.1 The Tsunogai derivations ϵ_k

In this section we write Lie$[a, b]$ for the fundamental Lie algebra associated to a once-punctured torus. This is a free Lia algebra on two generators and thus isomorphic to Lie$[x, y]$, but we prefer to distinguish the letters used because the topological fundamental group of a thrice-punctured sphere maps non-trivially to that of a once-punctured torus when two of the holes are joined together. We also have a natural map between the pro-unipotent fundamental groups, which gives a natural but highly non-trivial Lie algebra morphism

$$\mathrm{Lie}[x,y] \to \mathrm{Lie}[a,b] \tag{5.1}$$

between the associated graded Lie algebras (see (5.29) below).

We write $\mathrm{Der}^0\mathrm{Lie}[a,b]$ for the subspace of Lie algebra derivations of $\mathrm{Lie}[a,b]$ which annihilate the bracket $[a,b] = ab - ba$, where the last expression is valued in $\mathbb{Q}\langle a,b\rangle$. A derivation in $\mathrm{Der}^0\mathrm{Lie}[a,b]$ is entirely determined by its value on a (see for example Thm. 2.1 of [68] giving an explicit formula for the value of such a derivation on b).

Definition 5.1.1. Let $\delta \in \mathrm{Der}^0\mathrm{Lie}[a,b]$. We say that δ is of *homogeneous degree* n if $\delta(a)$ (and thus also $\delta(b)$) is a Lie polynomial of homogeneous degree $n+1$, i.e. if δ adds n to the degree of any polynomial it acts on. We furthermore assign *a-degree k and b-degree ℓ* to δ if $\delta(a)$ is a Lie polynomial of homogeneous degree $k+1$ in a and ℓ in b, in which case $\delta(b)$ is necessarily of a-degree k and b-degree $\ell+1$ (unless it vanishes). The b-degree of a derivation and the homogeneous b-degree of a polynomial in a,b is also referred to as the *depth*. The (homogeneous) degree of δ is equal to the sum of its a- and its b-degree.

We now need to introduce the *Tsunogai derivations* which were introduced by Tsunogai in 1995 [69], also see [70].

Definition 5.1.2. For all $i \geq 0$, let ϵ_{2i} denote the derivation of $\mathrm{Lie}[a,b]$ defined by

$$\epsilon_{2i}(a) = \mathrm{ad}_a^{2i}(b)\,, \qquad \epsilon_{2i}([a,b]) = 0\,, \qquad i \geq 0\,. \tag{5.2}$$

These two conditions determine ϵ_{2i} completely: its action on b is given explicitly by

$$\epsilon_0(b) = 0 \quad \text{and} \quad \epsilon_{2i}(b) = \sum_{j=0}^{i-1}(-1)^j \left[\mathrm{ad}_a^j(b), \mathrm{ad}_a^{2i-1-j}(b)\right]\,, \qquad i \geq 1\,. \tag{5.3}$$

We write $\mathfrak{u}$ for the Lie algebra of derivations of $\mathrm{Lie}[a,b]$ generated by the ϵ_{2i} for $i \geq 0$; the ϵ_{2i} are also called *geometric derivations*.

The Lie algebra $\mathfrak{u}$ of geometric derivations ϵ_{2i} has a rich history dating back to pioneering work of Ihara [71], with detailed studies in the work of Tsunogai [69,70]. They have become ubiquitous in the theory of elliptic MZVs (see for example [72,20,73,74,21,75] and [26]), with numerous references in the recent mathematics and string-theory literature. The derivations ϵ_0 and ϵ_2 defined in (5.2) play a special role. The derivation ϵ_0 is nilpotent on the ϵ_k (with even $k \geq 2$) in the sense that $\mathrm{ad}_{\epsilon_0}^{k-1}(\epsilon_k) = 0$, see part (i) of Lemma 5.1.5 below. The derivation ϵ_2 is central in $\mathrm{Der}^0\mathrm{Lie}[a,b]$ and will play no role in our construction.

We will also make essential use of the following $\mathfrak{sl}_2$-subalgebra of $\mathrm{Der}^0\mathrm{Lie}[a,b]$:

Definition 5.1.3. Define derivations $\epsilon_0^\vee, \mathrm{h} \in \mathrm{Der}^0\mathrm{Lie}[a,b]$ by

$$\epsilon_0^\vee(a) = 0\,, \qquad \epsilon_0^\vee(b) = a\,, \qquad \mathrm{h} = [\epsilon_0, \epsilon_0^\vee]\,. \tag{5.4}$$

The derivations ϵ_0, $\epsilon_0^\vee$ and h generate the Lie subalgebra of $\mathrm{Der}^0\mathrm{Lie}[a,b]$ denoted $\mathfrak{sl}_2$. The generator h satisfies $\mathrm{h}(a) = -a$ and $\mathrm{h}(b) = b$. We refer to vectors that are annihilated by ϵ_0 as *highest-weight vectors* and vectors that are annihilated by $\epsilon_0^\vee$ as *lowest-weight vectors*, respectively.

Definition 5.1.4. We will also need to introduce the *switch* operator θ, which can be considered as the automorphism of $\mathbb{Q}\langle\langle a,b\rangle\rangle$ that exchanges a and b, mapping a polynomial $f = f(a,b)$ to $\theta(f)$ with $[\theta(f)](a,b) = f(b,a)$, but also acts on derivations δ of $\mathbb{Q}\langle a,b\rangle$ by conjugation via the formula

$$\theta(\delta) \coloneqq \theta \circ \delta \circ \theta^{-1}\,, \tag{5.5}$$

i.e.

$$[\theta(\delta)](a) = \theta\big(\delta(b)\big)\,, \qquad [\theta(\delta)](b) = \theta\big(\delta(a)\big)\,. \tag{5.6}$$

Notice that $\theta(\epsilon_0) = \epsilon_0^\vee$ and therefore $\theta(\mathrm{h}) = -\mathrm{h}$.

The interplay of the derivations ϵ_k with with the $\mathfrak{sl}_2$-algebra and the switch operation θ in the previous definitions is reviewed in the following lemma (see for instance [69, 21, 26]).

Lemma 5.1.5. *For even values $k \geq 2$ and even or odd $j \geq 0$, set*

$$\epsilon_k^{(j)} \coloneqq \mathrm{ad}_{\epsilon_0}^j(\epsilon_k) \tag{5.7}$$

including $\epsilon_k^{(0)} = \epsilon_k$. Then the $\epsilon_k^{(j)}$ for $k \geq 2$ together with the generators $\epsilon_0, \epsilon_0^\vee, \mathrm{h}$ of the $\mathfrak{sl}_2$ in Definition 5.1.3 satisfy the following properties:

(i) The derivation $\epsilon_k^{(j)}$ is of a-degree $k-j-1$ and b-degree $j+1$ for $0 \leq j \leq k-2$ (in other words $\epsilon_k^{(j)}(a)$ is a polynomial of homogeneous a-degree $k-j$ and b-degree $j+1$) and thus of homogeneous degree k. We have the nilpotency property

$$\epsilon_k^{(j)} = 0 \quad \forall\ j > k-2\,. \tag{5.8}$$

The $\epsilon_k^{(k-2)}$ at maximum value of j are highest-weight vectors of the $\mathfrak{sl}_2$.

(ii) The derivations ϵ_k with $k \geq 2$ commute with $\epsilon_0^\vee$:

$$[\epsilon_0^\vee, \epsilon_k] = 0 \quad \forall\ k \geq 2\,, \tag{5.9}$$

i.e. they furnish lowest-weight vectors of $\mathfrak{sl}_2$.

(iii) The generator h of $\mathfrak{sl}_2$ satisfies the following commutation relations:

$$[\mathrm{h}, \epsilon_k] = (2-k)\epsilon_k \quad \forall\ k \geq 0\,, \qquad [\mathrm{h}, \epsilon_0^\vee] = -2\epsilon_0^\vee\,. \tag{5.10}$$

In particular this implies that the $\epsilon_k^{(j)}$ are all eigenvectors for h, with eigenvalues given by

$$[\mathrm{h}, \epsilon_k^{(j)}] = (2+2j-k)\epsilon_k^{(j)} \quad \forall\ k \geq 2\,,\ 0 \leq j \leq k-2\,. \tag{5.11}$$

(iv) The commutation relations of the $\mathfrak{sl}_2$ generators with $\epsilon_k^{(j)}$ at $k \geq 2$ and $0 \leq j \leq k-2$ are $[\epsilon_0, \epsilon_k^{(j)}] = \epsilon_k^{(j+1)}$ by definition, $[\mathrm{h}, \epsilon_k^{(j)}] = (2j+2-k)\epsilon_k^{(j)}$ by the previous point and

$$[\epsilon_0^\vee, \epsilon_k^{(j)}] = j(k-1-j)\epsilon_k^{(j-1)} . \tag{5.12}$$

(v) The switch operator in Definition 5.1.4 acts on the $\epsilon_k^{(j)}$ with $k \geq 2$ and $0 \leq j \leq k-2$ via

$$\theta\big(\epsilon_k^{(j)}\big) = -\frac{j!}{(k-2-j)!}\epsilon_k^{(k-2-j)} . \tag{5.13}$$

Proof. (i) The derivation ϵ_k is of a-degree $k-1$ and b-degree 1 by definition, and each application of ad_{ϵ_0} increases the b-degree by 1 without changing the total degree, so it decreases the a-degree by 1, proving the first statement. For the second statement, it is enough to show that $\epsilon_k^{(k-1)} = 0$ even though since $\epsilon_k^{(j)}$ shifts the (a, b) degrees of any polynomial in a, b by $(k-1-j, 1+j)$, the case $\epsilon_k^{(k-1)}$ of interest has (a, b) degrees $(0, k)$ as a derivation, meaning that a priori $\epsilon_k^{(k-1)}(a)$ could be a polynomial of a-degree 1 and b-degree k. Since the only Lie polynomial with these degrees is $\mathrm{ad}_b^k(a)$ up to scalar multiple, we must have

$$\epsilon_k^{(k-1)}(a) = c \cdot \mathrm{ad}_b^k(a) \tag{5.14}$$

for some constant c, and $\epsilon_k^{(k-1)}(b) = 0$. However, the derivation $\epsilon_k^{(k-1)}$ must annihilate the commutator $[a, b]$ since both ϵ_k and ϵ_0 do, so by the above, we have $\epsilon_k^{(k-1)}([a, b]) = c\cdot[\mathrm{ad}_b^k(a), b]$ which only vanishes for $c = 0$. Thus $c = 0$, so the derivation $\epsilon_k^{(k-1)} = 0$.

(ii) is readily established by evaluating $[\epsilon_0^\vee, \epsilon_{2i}] = \epsilon_0^\vee \epsilon_{2i} - \epsilon_{2i}\epsilon_0^\vee$ on a and b. The least straightforward part of the computation is to note that $\epsilon_0^\vee \sum_{j=0}^{i-1}(-1)^j[\mathrm{ad}_a^j(b), \mathrm{ad}_a^{2i-1-j}(b)]$ receives a single contribution from the $j = 0$ term, resulting in $[\epsilon_0^\vee(b), \mathrm{ad}_a^{2i-1}(b)] = \epsilon_{2i}(a)$.

(iii) Any monomial in a, b is an eigenvector for h, with the difference of the b-degree minus the a-degree as its eigenvalue. Since ϵ_k at $k \geq 0$ and $\epsilon_0^\vee$ shift the (a, b)-degrees by $(k-1, 1)$ and $(1, -1)$, respectively, the associated differences "b-degree minus a-degree" are shifted by $2-k$ in case of ϵ_k and -2 in case of $\epsilon_0^\vee$. This implies both identities in (5.10) as eigenvalue equations. The second claim (5.11) is a corollary which can for instance be inferred from $\epsilon_k^{(j)}$ shifting the (a, b)-degrees by $(k-1-j, j+1)$.

(iv) One can conveniently prove (5.12) by induction in j, starting with $[\epsilon_0^\vee, \epsilon_k^{(0)}] = 0$ as a base case which follows from (ii). The inductive step relies on the Jacobi identity $[\epsilon_0^\vee, \epsilon_k^{(j)}] = [\epsilon_0^\vee, [\epsilon_0, \epsilon_k^{(j-1)}]] = [[\epsilon_0^\vee, \epsilon_0], \epsilon_k^{(j-1)}] + [\epsilon_0, [\epsilon_0^\vee, \epsilon_k^{(j-1)}]]$ as well as (5.11) to evaluate the first term $[[\epsilon_0^\vee, \epsilon_0], \epsilon_k^{(j-1)}] = -[\mathrm{h}, \epsilon_k^{(j-1)}]$.

(v) We proceed by induction in j, first proving $\theta(\epsilon_k) = -\frac{1}{(k-2)!}\epsilon_k^{(k-2)}$ as a base case of (5.13) at $j = 0$.

Base case: If a derivation of degree > 0 annihilates the bracket $[a, b]$, then knowing its value on one of the variables a or b determines it completely. Hence, it suffices to show that

$\theta(\epsilon_k)$ and $-\frac{1}{(k-2)!}\epsilon_k^{(k-2)}$ have the same action on b to establish their equality as derivations in $\mathrm{Der}^0\mathrm{Lie}[a,b]$. For this purpose, we successively simplify

$$\begin{aligned}\epsilon_k^{(k-2)}(b) &= (\epsilon_0)^{k-2}\epsilon_k(b) = \sum_{j=0}^{\frac{k}{2}-1}(-1)^j(\epsilon_0)^{k-2}\left[\mathrm{ad}_a^j(b),\mathrm{ad}_a^{k-1-j}(b)\right] \\ &= (\epsilon_0)^{k-2}\left[b,\mathrm{ad}_a^{k-1}(b)\right] = -\left[b,(\epsilon_0)^{k-2}\mathrm{ad}_a^{k-2}([b,a])\right] \\ &= -(k-2)!\left[b,\mathrm{ad}_b^{k-2}([b,a])\right] = -(k-2)!\,\mathrm{ad}_b^k(a)\,. \end{aligned} \tag{5.15}$$

In the first step, we have used $\epsilon_0(b)=0$ to remove all contributions to $\epsilon_k^{(k-2)}(b)$ with an ϵ_0 on the right of ϵ_k. The second step makes use of the expression (5.3) for $\epsilon_k(b)$ and k even. The third step relies on the fact that for $m\geq 1$, $\mathrm{ad}_a^m(b)$ is annihilated by $(\epsilon_0)^m$ such that $[\mathrm{ad}_a^j(b),\mathrm{ad}_a^{k-1-j}(b)]$ is annihilated by $(\epsilon_0)^{k-2}$ unless $j=0$. After redistributing the $(k-1)$-fold action of ad_a in the fourth step, we note in the fifth step that the $k-2$ factors of ϵ_0 can act on the $k-2$ exposed powers of ad_a (besides $[b,a]$ which is annihilated by ϵ_0) in $(k-2)!$ different permutations, converting ad_a^{k-2} to ad_b^{k-2} in all cases. The end result of (5.15) after repackaging the powers of ad_b is equivalent to

$$\epsilon_k^{(k-2)}(b) = -(k-2)!\,\mathrm{ad}_b^k(a) = -(k-2)!\,\theta\big(\epsilon_k(a)\big) \tag{5.16}$$

by virtue of (5.2). As a consequence, $\theta(\epsilon_k)$ and $-\frac{1}{(k-2)!}\epsilon_k^{(k-2)}$ have the same action on b and must agree as derivations since they both annihilate $[a,b]$ and have degree >0.

Inductive step: Now we can take care of (5.13) at values $j>0$ by induction as follows:

$$\begin{aligned}\theta(\epsilon_k^{(j)}) &= \theta\big([\epsilon_0,\epsilon_k^{(j-1)}]\big) = \big[\theta(\epsilon_0),\theta(\epsilon_k^{(j-1)})\big] = -\frac{(j-1)!}{(k-1-j)!}\big[\epsilon_0^\vee,\epsilon_k^{(k-1-j)}\big] \\ &= -\frac{(j-1)!}{(k-1-j)!}j(k-1-j)\epsilon_k^{(k-2-j)} = -\frac{j!}{(k-2-j)!}\epsilon_k^{(k-2-j)}\,, \end{aligned} \tag{5.17}$$

where we used $\theta(\epsilon_0)=\epsilon_0^\vee$ and the induction hypothesis $\theta(\epsilon_k^{(j-1)}) = -\frac{(j-1)!}{(k-1-j)!}\epsilon_k^{(k-1-j)}$ in the third step and (5.12) proven as (iv) in passing to the second line. ☐

Remark 5.1.6. Note that the $\epsilon_k^{(j)}$ are by no means free generators of $\mathfrak{u}$; commutators of two or more of them obey a number of relations related to period polynomials of holomorphic cusp forms on $\mathrm{SL}_2(\mathbb{Z})$, the first of which were noticed by Ihara and Takao (cf. [24]). The relations between brackets of two ϵ_k's were classified in [25] where the connection with cusp forms was made explicit; subsequently Pollack in [26] unearthed many more relations, and made a general conjecture about the full set of relations between the $\epsilon_k^{(j)}$. These relations, which we call *Pollack's relations*, were proved to be motivic in [21]. They appear in many works related to elliptic MZVs, such as for example [76] and [74]. The lowest-degree Pollack relations arise in degrees 14 and 16, and are given by

$$0 = [\epsilon_4,\epsilon_{10}] - 3[\epsilon_6,\epsilon_8]\,, \tag{5.18}$$

$$
\begin{aligned}
0 = 80[\epsilon_4^{(1)}, \epsilon_{12}] + 16[\epsilon_{12}^{(1)}, \epsilon_4] - 250[\epsilon_6^{(1)}, \epsilon_{10}] - 125[\epsilon_{10}^{(1)}, \epsilon_6] + 280[\epsilon_8^{(1)}, \epsilon_8] \\
- 462[\epsilon_4, [\epsilon_4, \epsilon_8]] - 1725[\epsilon_6, [\epsilon_6, \epsilon_4]] \,.
\end{aligned}
\tag{5.19}
$$

5.2 The genus one motivic Lie algebra

In [21], Hain and Matsumoto define a Tannakian category MEM of *mixed elliptic motives* and study its fundamental Lie algebra. We do not recall their construction here, but restrict ourselves to giving the main result of their article that we will use here. Let $\mathrm{Lie}\,\pi_1(MEM)$ denote the graded Lie algebra associated to the unipotent radical of the fundamental group of the category MEM. Let $\mathfrak{sl}_2$ denotes the Lie subalgebra of $\mathrm{Der}^0\mathrm{Lie}[a,b]$ from Definition 5.1.3.

Theorem 5.2.1 (Hain–Matsumoto)**.** *There is a Lie algebra morphism (the "monodromy representation", see section 22 of [21])*

$$
\mathrm{Lie}\,\pi_1(MEM) \to \mathrm{Der}^0\mathrm{Lie}[a,b] \tag{5.20}
$$

whose image $\mathcal{L}$ is generated by the derivations $\epsilon_k^{(j)}$ for even $k > 0$ and $0 \le j \le k-2$ together with derivations σ_w for each odd $w \ge 3$, and has the following properties:

(i) The Lie subalgebra $\mathcal{S} \coloneqq \mathrm{Lie}[\sigma_3, \sigma_5, \ldots] \subset \mathcal{L}$ is free,

(ii) The Lie subalgebra $\mathfrak{u}$ generated by the $\epsilon_k^{(j)}$ is normal in $\mathcal{L}$, i.e. $\mathcal{L} = \mathfrak{u} \rtimes \mathcal{S}$,

(iii) $\mathcal{L}$ is an $\mathfrak{sl}_2$-module, and $\mathfrak{u}$ is also an $\mathfrak{sl}_2$-module,

(iv) the Lie subalgebra $\mathfrak{u} \rtimes \mathfrak{sl}_2$ is normal inside $\mathcal{L} \rtimes \mathfrak{sl}_2$.

Remark 5.2.2. Although entirely phrased in terms of the monodromy representation of the fundamental Lie algebra of the category MEM, this theorem reflects essential geometric/arithmetic content. The quotient of $\mathcal{L}$ by the normal Lie subalgebra $\mathfrak{u}$ is isomorphic to $\mathcal{S}$, which is itself free on one generator in each odd rank ≥ 3, i.e. isomorphic to $\mathrm{Lie}\,\pi_1(MTM)$ the fundamental Lie algebra of the category of mixed Tate motives unramified over $\mathbb{Z}$, and this reflects the fact geometrically expressed by the degeneration of an elliptic curve parametrized by τ to the nodal elliptic curve by letting τ tend to $i\infty$ (see appendix A).

To be more precise, if one considers the universal elliptic curve $\mathcal{E}$ as a fibration over the Deligne–Mumford compactification $\overline{\mathcal{M}}_{1,1}$ of the moduli space of elliptic curves $\mathcal{M}_{1,1}$ (viewed as the usual fundamental domain for the action of $\mathrm{SL}_2(\mathbb{Z})$ on the Poincaré upper half-plane, parametrized by the variable τ), then the fiber over $\tau = i\infty$ is the so-called nodal (or degenerate) elliptic curve E_∞. Let π_1 denote the fundamental group of the punctured torus, freely generated by loops α and β through and around the genus hole, and let $\hat{\pi}_1$ be its profinite completion. Then there is a canonical *arithmetic* outer Galois action of the absolute Galois group $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ on $\hat{\pi}_1(E_\infty)$. Furthermore, since $\mathcal{E}$ is a fibration over the base $\mathcal{M}_{1,1}$ with an elliptic curve as a fiber, $\pi_1(\mathcal{E})$ fits into a short exact sequence whose kernel is free on two generators (the π_1 of the fiber) and whose quotient is $\mathrm{SL}_2(\mathbb{Z})$ (the π_1 of the base), and thus there is a second, *geometric* outer group action on $\pi_1(E_\infty)$ by the group $\mathrm{SL}_2(\mathbb{Z})$, which extends to an action of the profinite completion $\widehat{\mathrm{SL}_2}(\mathbb{Z})$ on $\hat{\pi}_1(E_\infty)$. Thus we have two disjoint profinite groups, $\widehat{\mathrm{SL}_2}(\mathbb{Z})$ and the absolute Galois group $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ [77], acting as automorphism groups of $\hat{\pi}_1(E_\infty)$.

The pro-unipotent version of this situation, or rather the associated Lie algebra version, has $\mathcal{S} = \mathrm{Lie}\,\pi_1(MTM)$ playing the role of $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ and $\mathfrak{u} \rtimes \mathrm{sl}_2$ playing the role of $\mathrm{SL}_2(\mathbb{Z})$, both acting as derivation Lie algebras (the Lie algebra version of automorphism groups) of $\mathrm{Lie}[a, b]$, the free Lie algebra on two generators which plays the role of $\hat{\pi}_1(E_\infty)$. The fact that $\mathcal{S}$ acts on $\mathfrak{u} \rtimes \mathfrak{sl}_2$ reflects the fact that $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ acts not only on $\hat{\pi}_1(E_\infty)$ but also on $\widehat{\mathrm{SL}_2}(\mathbb{Z})$, since the latter group is also a fundamental group, namely of $\mathcal{M}_{1,1}$.

Hain and Matsumoto conjecture that the surjective morphism from $\mathrm{Lie}\,\pi_1(MEM)$ to $\mathcal{L}$ is actually an isomorphism, but this is still an open question. They further explain that there is a natural surjection from $\mathrm{Lie}\,\pi_1(MEM)$ to $\mathrm{Lie}\,\pi_1(MTM)$, the fundamental Lie algebra of the category of mixed Tate motives unramified over $\mathbb{Z}$. Since this category was shown by Brown to be generated by the motivic MZVs, we have the isomorphism

$$\mathrm{Lie}\,\pi_1(MTM) = \mathfrak{mz}^\vee\,, \tag{5.21}$$

where $\mathfrak{mz}^\vee$ is the Lie algebra associated to the motivic MZVs. Hain and Matsumoto further proved the existence of a section map

$$\mathrm{Lie}\,\pi_1(MTM) \hookrightarrow \mathrm{Lie}\,\pi_1(MEM)\,, \tag{5.22}$$

which explains the semi-direct product structure in (ii), with the image of $\mathrm{Lie}\,\pi_1(MTM)$ identified with $\mathcal{S} \subset \mathrm{Lie}\,\pi_1(MEM)$. The section map was defined explicitly in independent parallel work by Enriquez in [20], working with the *Grothendieck–Teichmüller Lie algebra* $\mathfrak{grt}$. Thanks to this work, $\mathcal{S}$ is identified as a canonical Lie subalgebra of $\mathcal{L}$. However, neither Hain–Matsumoto nor Enriquez gave a canonical choice of the actual generators σ_w for odd $w \geq 3$; a priori, the choice of generator σ_w is only defined up to adding on brackets of σ_u with smaller $u < w$. This exactly parallels the fact that no special set of free generators of the motivic Lie algebra $\mathrm{Lie}\,\pi_1(MTM) = \mathfrak{mz}^\vee$ was defined prior to the canonical family of g_w in genus zero defined in section 3.3.

Our main purpose in this section is to point out that, thanks to the canonical genus zero generators g_w and the existence of the section map (5.22), we can now define a canonical choice of genus one generators σ_w simply as the images of the g_w under the section map. More precisely, we will construct an explicit Lie algebra morphism

$$\tilde{\gamma} : \mathfrak{mz}^\vee \to \mathrm{Lie}[\sigma_3, \sigma_5, \ldots,] \subset \mathrm{Der}^0\mathrm{Lie}[a, b] \tag{5.23}$$

and use it to define the σ_w (as images of the g_w), to compute them and to determine many of their properties. In the same way as the Ihara derivations of g_w are called zeta generators in genus zero, we will refer to the σ_w as *zeta generators in genus one*. The tight interplay of zeta generators in genus zero and one can for instance be seen from (5.41) below where the action of σ_w is computed from g_w. Additional facets of the relation between zeta generators in genus zero and genus one can be found in appendix A.

Let us show how the map $\tilde{\gamma}$ in (5.23) relates to the Grothendieck–Teichmüller section map defined by Enriquez. We do not need to give the definition of $\mathfrak{grt}$ here, but only to mention two essential properties that we need: firstly, there is an injective morphism

$$\begin{aligned} \mathfrak{mz}^\vee &\hookrightarrow \mathfrak{grt}\,, \\ h(x,y) &\mapsto h(x,-y)\,, \end{aligned} \tag{5.24}$$

(this is a direct consequence of the fact that Goncharov's motivic MZVs satisfy the associator relations, see for example [78]) and secondly, Enriquez [20] defined an injective map

$$\mathfrak{grt} \hookrightarrow \mathrm{Der}^0\mathrm{Lie}[a,b] \tag{5.25}$$

which was shown in [23] to be equivalent to the Hain–Matsumoto section, using methods from Écalle's mould theory that will be explained in section 6 below. Let

$$\gamma : \mathfrak{mz}^\vee \hookrightarrow \mathrm{Der}^0\mathrm{Lie}[a,b] \tag{5.26}$$

denote the composition of (5.24) with (5.25). The explicit isomorphism $\tilde{\gamma}$ announced in (5.23) is given by

$$\tilde{\gamma} = \theta \circ \gamma\,, \tag{5.27}$$

where θ is the switch automorphism of $\mathbb{Q}\langle\langle a,b\rangle\rangle$ exchanging a and b, see Definition 5.1.4.

Definition 5.2.3. Let g_w for odd $w \geq 3$ denote the family of canonical free generators of $\mathfrak{mz}^\vee$ given in Definition 3.3.4. Set

$$\tau_w \coloneqq \gamma(g_w)\,, \qquad \sigma_w \coloneqq \tilde{\gamma}(g_w)\,, \tag{5.28}$$

where γ is as in (5.26) and $\tilde{\gamma}$ as in (5.27). This definition accomplishes the second goal of this article of giving a canonical choice for the zeta generators σ_w in genus one for odd $w \geq 3$.

The remainder of section 5 and all of sections 6 and 7 are devoted to the study of the canonical zeta generators σ_w in genus one. Section 5.3 gives an explicit step-by-step construction of the Enriquez map (5.25), and in Theorem 5.4.1 of section 5.4 we list several properties of the zeta generators σ_w and their switch images τ_w. Section 5.5 contains the low-degree parts of σ_w for $w = 3,5,7,9$. The proofs of some of the properties in Theorem 5.4.1 rely on a second, mould theoretic construction of the map γ, which is given in section 6.1 along with a necessary introduction to mould theory; the full proof of the theorem is contained in section 6.2 (using mould theory), section 6.3 (using the $\mathfrak{sl}_2$ subalgebra of Definition 5.1.3) and section 7.1 (summarizing the essential argument of [79, 21]). Section 7.3 introduces a recursive procedure to compute high-degree contributions to σ_w in terms of ϵ_k which leads to a variety of explicit results beyond the state-of-the-art in section 7.4.

5.3 Genus one derivations from genus zero polynomials

Since in this section we will work only in odd weights w, we can work entirely mod ζ_2, in the $\mathbb{Q}$-algebras $\overline{\mathcal{FZ}}$ and $\overline{\mathcal{MZ}}$.

The surjection $\mathcal{FZ} \twoheadrightarrow \mathcal{MZ}$ from section 2.2 induces a surjection $\overline{\mathcal{FZ}} \twoheadrightarrow \overline{\mathcal{MZ}}$ and a surjection $\mathfrak{fz} \twoheadrightarrow \mathfrak{mz}$. As we saw in the previous sections, we can pass to the dual spaces using the Z-map and these surjections induce injections $\mathfrak{mz}^\vee \hookrightarrow \mathfrak{fz}^\vee = \mathfrak{ds}$ and $\overline{\mathcal{MZ}}^\vee \hookrightarrow \overline{\mathcal{FZ}}^\vee = \mathcal{U}\mathfrak{ds}$ in the dual spaces. The complete situation combining all the surjections, dual inclusions and Z-maps is summarized in the diagram (3.25).

The map from g_w to σ_w is to be viewed as a map from genus zero to genus one. The genus zero situation here is represented by the Lie algebra $\mathrm{Lie}[x,y]$, which is identified with the graded Lie algebra associated to the pro-unipotent completion of the fundamental group π_1 of the sphere with three punctures (which is free on two generators). The genus one situation is represented by the completion $\widehat{\mathrm{Lie}}[a,b] \subset \mathbb{Q}\langle\langle a,b\rangle\rangle$ of the free Lie algebra on two generators $\mathrm{Lie}[a,b]$, the graded Lie algebra of the pro-unipotent fundamental group of the once-punctured torus. The topological map from the sphere to the torus obtained by joining two of the punctures passes to the topological fundamental groups, their unipotent completions and then via formality isomorphisms to the corresponding graded Lie algebras, yielding the following Lie algebra morphism:

$$\begin{aligned} \psi : \mathrm{Lie}[x,y] &\to \widehat{\mathrm{Lie}}[a,b]\,, \\ x &\mapsto t_{12}\,, \\ y &\mapsto t_{01}\,, \end{aligned} \tag{5.29}$$

where letting B_n denote the standard Bernoulli numbers,

$$\begin{aligned} t_{01} &:= \frac{\mathrm{ad}_b}{e^{\mathrm{ad}_b}-1}(-a) = -a - \sum_{n\geq 1}\frac{\mathrm{B}_n}{n!}\mathrm{ad}_b^n(a) = -a + \tfrac{1}{2}\mathrm{ad}_b(a) - \tfrac{1}{12}\mathrm{ad}_b^2(a) + \tfrac{1}{720}\mathrm{ad}_b^4(a) + \dots\,, \\ t_{12} &:= [a,b]\,. \end{aligned} \tag{5.30}$$

The map ψ in (5.29) also arises when computing the Knizhnik–Zamolodchikov–Bernard connection on a degeneration limit of the torus (corresponding topologically to the degenerate torus obtained by joining two punctures of the thrice-punctured sphere), and matching the result with the Knizhnik–Zamolodchikov connection on the sphere. This calculation is spelled out in detail in appendix A.

In order to explicitly define the map γ in (5.26), we will make use of the notion of a *partner* [23]: for any $g(a,b) \in \mathrm{Lie}[a,b]$, we write $g = g_a a + g_b b$ and define the partner of g by the formula

$$g' := \sum_{i\geq 0}\frac{(-1)^{i-1}}{i!}a^i b\, \partial_a^i\big(g_a\big) \in \mathbb{Q}\langle a,b\rangle\,, \tag{5.31}$$

where ∂_a is the derivation of $\mathbb{Q}\langle\langle a,b\rangle\rangle$ defined by $\partial_a(a)=1$ and $\partial_a(b)=0$. It is shown in Lemma 2.1.1 of [23] that the derivation $a\mapsto g$, $b\mapsto g'$ lies in $\mathrm{Der}^0\mathrm{Lie}[a,b]$ if and only if g has a certain property called *push-invariance* to which we will return in section 6 (see (6.21)).

We can now proceed to the explicit definition of the map γ of (5.26). Define $\tau_h \coloneqq \gamma(h) \in \mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$ to be the derivation obtained from $h \in \mathfrak{mz}^\vee$ by the following procedure:

- Let $h = h(x,y)$ be in $\mathfrak{mz}^\vee$ and define a derivation κ_h of the Lie subalgebra $\mathrm{Lie}[t_{12}, t_{01}] \subset \widehat{\mathrm{Lie}}[a,b]$ by[8]

$$\kappa_h(t_{12}) = 0\,, \qquad \kappa_h(t_{01}) = [t_{01}, h(t_{12}, -t_{01})]\,. \tag{5.32}$$

- By the "extension lemma" 2.1.2 of [23], there exists a unique derivation τ_h of $\mathbb{Q}\langle\langle a,b\rangle\rangle$ having the following two properties: firstly

$$\tau_h(t_{01}) = \kappa_h(t_{01})\,, \tag{5.33}$$

and secondly $\tau_h(b)$ is (in each degree) the *partner* of $\tau_h(a)$ as defined in (5.31).

Specifically, the action of the derivation τ_h on a can be inferred from (5.33) degree by degree as follows. Suppose $h(x,y)$ is homogeneous of degree w in x, y. We have from (5.30)

$$\tau_h(t_{01}) = \tau_h\big(-a + \tfrac{1}{2}[b,a] - \tfrac{1}{12}[b,[b,a]] + \cdots\big) \tag{5.34}$$

so

$$\tau_h(a) = -\kappa_h(t_{01}) + \tfrac{1}{2}\tau_h\big([b,a]\big) - \tfrac{1}{12}\tau_h\big([b,[b,a]]\big) + \cdots \tag{5.35}$$

since $\tau_h(t_{01}) = \kappa_h(t_{01})$. In particular, the lowest degree part of $\tau_h(a)$ is equal to the lowest degree part of $-\kappa_h(t_{01})$, which is equal to $[a, h^d([a,b],a)]$ from (5.32) and where d denotes the minimal x-degree of h and $h^d(x,y)$ are the contributions to $h(x,y)$ of x-degree d; the term $[a, h^d([a,b],a)]$ is of degree $w+d+1$ in a, b. So we have

$$\tau_h(a)_{w+d+1} = -\kappa_h(t_{01})_{w+d+1} = [a, h^d([a,b],a)] \tag{5.36}$$

in lowest degree, where g_d denotes the degree-d contributions to polynomials g in a and b. We set $\tau_h(b)_{w+d+1}$ to be the partner of $\tau_h(a)_{w+d+1}$ using the formula (5.31).

We then use (5.35) to recursively compute $\tau_h(a)$ in successive degrees $w+d+i$ $(i > 1)$:

$$\begin{aligned}
\tau_h(a)_{w+d+2} &= -\kappa_h(t_{01})_{w+d+2} + \tfrac{1}{2}[\tau_h(b)_{w+d+1}, a] + \tfrac{1}{2}[b, \tau_h(a)_{w+d+1}]\,,\\
\tau_h(a)_{w+d+3} &= -\kappa_h(t_{01})_{w+d+3} + \tfrac{1}{2}[\tau_h(b)_{w+d+2}, a] + \tfrac{1}{2}[b, \tau_h(a)_{w+d+2}]\\
&\quad - \tfrac{1}{12}[\tau_h(b)_{w+d+1}, [b,a]] - \tfrac{1}{12}[b, [\tau_h(b)_{w+d+2}, a]] - \tfrac{1}{12}[b, [b, \tau_h(a)_{w+d+1}]]\,,\\
&\text{etc.}\,,
\end{aligned} \tag{5.37}$$

defining $\tau_h(b)_{w+d+i}$ to be the partner of $\tau_h(a)_{w+d+i}$ at each successive degree via (5.31). This process yields a unique Lie series $\tau_h(a)$. As observed just after (5.31), if $\tau_h(a)$ has

[8] The minus sign in front of t_{01} in (5.32) is present because if $h(x,y) \in \mathfrak{mz}^\vee \subset \mathfrak{ds}$, then as in (5.24), the polynomial $h(x,-y)$ lies in $\mathfrak{grt}$. Since the process described in the present section is an explicit version of Enriquez's map (5.25) from $\mathfrak{grt}$ to $\mathrm{Der}^0\mathrm{Lie}[a,b]$, the starting point of the map is the $\mathfrak{grt}$ polynomial $h(x,-y)$, or more precisely, the associated Ihara derivation which maps $x \mapsto 0$ and $y \mapsto [y, h(x,-y)]$. The first step in the explicit construction of the Enriquez map is transporting this Ihara derivation to a derivation on $\mathrm{Lie}[t_{01}, t_{12}]$ via the map (5.29), which is what is expressed in (5.32).

the property of *push-invariance* then $\tau_h \in \mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$, so in particular τ_h annihilates $[a,b] = t_{12}$, and thus τ_h is an extension of κ_h to all of $\mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$. The fact that $\tau_h(a)$ does indeed possess the necessary property of push-invariance is proved in Theorem 6.1.6 (iii) below.

- For each $h \in \mathfrak{mz}^\vee$, we define $\sigma_h \in \mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$ to be the derivation obtained from τ_h by the switch operator in Definition 5.1.4: we set

$$\sigma_h = \theta(\tau_h)\,, \tag{5.38}$$

or equivalently, σ_h acts on a and b via

$$\sigma_h(a) = \theta\big(\tau_h(b)\big)\,, \qquad \sigma_h(b) = \theta\big(\tau_h(a)\big)\,. \tag{5.39}$$

Combining all the steps of the process above then yields explicit versions

$$\begin{aligned} \gamma : \mathfrak{mz}^\vee &\hookrightarrow \mathrm{Der}^0\mathrm{Lie}[a,b]\,, & \tilde{\gamma} : \mathfrak{mz}^\vee &\hookrightarrow \mathrm{Der}^0\mathrm{Lie}[a,b]\,, \\ h &\mapsto \tau_h\,, & h &\mapsto \sigma_h\,, \end{aligned} \tag{5.40}$$

of the maps γ from (5.26) and $\tilde{\gamma}$ from (5.23).

5.4 The canonical genus one derivations σ_w

We shall now specialize the above construction of $\gamma(h)$ and $\tilde{\gamma}(h)$ for general $h \in \mathfrak{mz}^\vee$ to the canonical polynomials $h \to g_w$ of Definition 3.3.4 for odd $w \geq 3$. The concrete realization of the maps $\gamma, \tilde{\gamma}$ in (5.40) provided by the previous section allows for an explicit computation of the zeta generators σ_w, τ_w in (5.28). By (5.32) and (5.39), the action of the genus one zeta generators $\sigma_w = \tilde{\gamma}(g_w)$ and on the smaller Lie subalgebra $\mathrm{Lie}[t_{01}, t_{12}] \subset \widehat{\mathrm{Lie}}[a,b]$ is given by

$$\sigma_w(t_{12}) = 0\,, \qquad \sigma_w(t_{01}) = \theta\big(\big[t_{01}, g_w(t_{12}, -t_{01})\big]\big)\,, \tag{5.41}$$

obtained from applying the switch θ to

$$\tau_w(t_{12}) = 0\,, \qquad \tau_w(t_{01}) = \big[t_{01}, g_w(t_{12}, -t_{01})\big]\,. \tag{5.42}$$

By the discussion in section 3.6, the canonical polynomials g_w are determined by the (modified) Drinfeld associator and the $\mathbb{Q}$ relations among MZVs. Hence, the information from iterated integrals in genus zero already fixes the defining relations (5.42) of zeta generators in genus one. Further discussions of the tight interplay between genus zero and genus one can be found in appendix A.

In the previous section, we explained how to infer $\tau_h(a)$ and $\tau_h(b)$ from $\tau_h(t_{01})$ and $\tau_h(t_{12})$ for general $h \in \mathfrak{mz}^\vee$ from (5.32) by the extension lemma 2.1.2 of [23]. To compute $\sigma_w(a)$ and $\sigma_w(b)$, we can either apply that method with $h = g_w$ and use the switch θ or use the same method directly from (5.41).

The derivations τ_w and σ_w associated to g_w for odd w have many remarkable properties, of which a number are listed in the following theorem. Several of these are statements for the different degree parts of τ_w and σ_w (where degree refers to the degree as a derivation). The degree $2w$ parts of τ_w and σ_w turn out to play a special role and are called the *key degree* parts $\tau_w^{\rm key}$ and $\sigma_w^{\rm key}$. In section 6.1 we will present a brief introduction to mould theory which will enable us to prove the first three of these in section 6.2; the others are proved in section 6.3. Part (i) and (ii) of the theorem below are already known from [23] and implicitly from [20, 21]. Part (iv) follows straightforwardly from Theorem 5.2.1 [21]. Part (v) is essentially in [21], see for instance Remark 20.4. The last two sentences of part (vi) readily follow from Theorem 5.2.1 as can be seen from their proof in section 6.3.2 below. Part (vii) was proven in section 27 of [21] as will be reviewed in section 7.1 below.

Theorem 5.4.1. *For odd $w \geq 3$, the zeta generators τ_w and σ_w in Definition 5.2.3 satisfy:*

(i) Both τ_w and σ_w lie in $\mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$.

(ii) The minimal degree of τ_w and σ_w is $w+1$, and all odd-degree terms are equal to zero. All terms of the power series $\tau_w(a)$ are of constant a-degree $w+1$, or equivalently (thanks to the switch), all terms of the power series $\sigma_w(a)$ have constant b-degree w.

(iii) Both τ_w and σ_w are entirely determined by their parts of degree $< 2w$.

(iv) There are no highest-weight vectors of $\mathfrak{sl}_2$ in σ_w beyond key degree.

(v) All contributions to τ_w and σ_w of degree different from $2w$ lie in $\mathfrak{u}$. The key-degree parts $\tau_w^{\rm key}$ and $\sigma_w^{\rm key}$ do not lie in $\mathfrak{u}$.

(vi) Define the arithmetic part *$z_w \in \mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$ of the derivation σ_w to be the one-dimensional component of $\sigma_w^{\rm key}$ as an $\mathfrak{sl}_2$ representation, i.e. which commutes with the generators $\epsilon_0, \epsilon_0^\vee$ of $\mathfrak{sl}_2 \subset \mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$ in Definition 5.1.3. Then, the difference $\sigma_w^{\rm key} - z_w$ and by (v) in fact all of $\sigma_w - z_w$ lies in $\mathfrak{u}$. Moreover, while the z_w themselves do not lie in $\mathfrak{u}$, the brackets $[z_w, \epsilon_k]$ for any even $k \geq 0$ lie in $\mathfrak{u}$.*

(vii) σ_w commutes with the infinite series N in geometric derivations defined by

$$N := -\epsilon_0 + \sum_{k=2}^{\infty} (2k-1) \frac{\mathrm{B}_{2k}}{(2k)!} \epsilon_{2k} \,. \tag{5.43}$$

Remark 5.4.2. As pointed out in [21, 6], the characterization of the arithmetic parts z_w in the earlier literature as commuting with $\mathfrak{sl}_2$ and not lying in $\mathfrak{u}$ does not identify the z_w uniquely; ambiguities remain for $w \geq 7$, since one can modify z_w by adding on $\mathfrak{sl}_2$-invariant combinations of $\epsilon_k^{(j)}$ in $\sigma_w^{\rm key} - z_w$ while keeping the overall σ_w unchanged (see for instance Remark 20.3 (ii) of [21]). In order to eliminate this ambiguity, we added the defining property in Theorem 5.4.1 (vi) that z_w exhausts the one-dimensional irreducible $\mathfrak{sl}_2$ representations of $\sigma_w^{\rm key}$ (or equivalently, $\sigma_w^{\rm key} - z_w$ contains no one-dimensional irreducible representations of

$\mathfrak{sl}_2$). Moreover, the canonical zeta generators σ_w established with the help of the polynomials $g_w(x,y)$ resolve an independent class of earlier ambiguities in z_w, namely it is no longer possible to add on nested brackets of lower-weight z_v with $v < w$ (e.g. for example, we cannot add a multiple of $[z_3,[z_3,z_5]]$ to z_{11}). Hence, the properties in part (vi) of Theorem 5.4.1 single out unique canonical arithmetic derivations z_w at each odd $w \geq 3$.

5.5 Expansions of σ_w in low degree

In this section we spell out the explicit low-degree parts of the σ_w up to $w=9$, in order to give a feel for their appearance (relegating a detailed discussion of computational methods to section 7.3). For this purpose, we rewrite the expansion of $\sigma_w(a)$ and $\sigma_w(b)$ resulting from (5.41) and the extension lemma in terms of the geometric derivations $\epsilon_k^{(j)}$ in (5.7) acting on a and b, up to the arithmetic parts z_w at key degree described in Theorem 5.4.1 (vi). Note that according to Theorem 5.4.1 (v), the "key degree" part $\sigma_w^{\rm key}$ of σ_w, which is the part in degree $2w$ (as a derivation) is the only part not consisting of brackets of $\epsilon_k^{(j)}$.

In section 5.5.3 below we give a more detailed description of the computation algorithm, but begin by presenting a few examples to convey an impression of the structure of the σ_w. In the following examples for $w=3,5,7$, we decompose $\sigma_w^{\rm key}$ into the unique choice of its $\mathfrak{sl}_2$ invariant part z_w in Theorem 5.4.1 (vi) and nested brackets of $\epsilon_k^{(j)}$ in (≥ 3)-dimensional irreducible representations of $\mathfrak{sl}_2$.

5.5.1 The case $w=3$

In this situation, we first give the complete calculation of the derivations τ_3 and σ_3 related by the switch, and specify the derivation z_3 by directly giving its values on a and b. Recall that the switch maps τ_w to σ_w via (5.39) and acts on the derivations $\epsilon_k^{(j)}$ according to (5.13). Direct computation based on (5.42) shows that

$$\begin{aligned}\tau_3 = \epsilon_4 + \tau_3^{\rm key} &- \tfrac{1}{960}[\epsilon_4^{(1)},\epsilon_4^{(2)}] + \tfrac{1}{725760}[\epsilon_4^{(1)},\epsilon_6^{(4)}] - \tfrac{1}{1451520}[\epsilon_4^{(2)},\epsilon_6^{(3)}]\\ &+ \tfrac{1}{1741824000}[\epsilon_4^{(2)},\epsilon_8^{(5)}] - \tfrac{1}{870912000}[\epsilon_4^{(1)},\epsilon_8^{(6)}] + \tfrac{1}{2786918400}[\epsilon_4^{(2)},[\epsilon_4^{(2)},\epsilon_6^{(4)}]]\\ &+ \tfrac{1}{1931334451200}[\epsilon_4^{(1)},\epsilon_{10}^{(8)}] - \tfrac{1}{3862668902400}[\epsilon_4^{(2)},\epsilon_{10}^{(7)}] + \ldots\,,\end{aligned} \tag{5.44}$$

with an infinite series in nested brackets of $\epsilon_{k_i}^{(j_i)}$ of total degree $\sum_i k_i \geq 16$ in the ellipsis. Here and in section 5.5.2 below, we have made a choice on how the Pollack relations of Remark 5.1.6 are used to represent the degree ≥ 14 terms of σ_w and τ_w.

The key-degree part $\tau_3^{\rm key}$ concentrated in degree 6 is given explicitly by

$$\begin{aligned}\tau_3^{\rm key}(a) &= -\tfrac{1}{4}[aaababb] - \tfrac{1}{4}[aaabbab] - \tfrac{1}{12}[aababab]\,,\\ \tau_3^{\rm key}(b) &= \tfrac{1}{4}[aababbb] + \tfrac{1}{4}[aabbabb] + \tfrac{1}{4}[aabbbab] + \tfrac{1}{12}[abababb]\,,\end{aligned} \tag{5.45}$$

where we employ the Lyndon-bracket notation introduced in Theorem 3.5.2.

Applying the switch (5.39) and (5.13) to τ_3 and $\tau_3^{\rm key}$, we obtain the following explicit formula for σ_3 (again skipping an infinity of contributions at degree $\sum_i k_i \geq 16$):

$$\begin{aligned}\sigma_3 = &-\tfrac{1}{2}\epsilon_4^{(2)} + z_3 + \tfrac{1}{480}[\epsilon_4,\epsilon_4^{(1)}] + \tfrac{1}{30240}[\epsilon_4^{(1)},\epsilon_6] - \tfrac{1}{120960}[\epsilon_4,\epsilon_6^{(1)}] + \tfrac{1}{7257600}[\epsilon_4,\epsilon_8^{(1)}] \\ &- \tfrac{1}{1209600}[\epsilon_4^{(1)},\epsilon_8] - \tfrac{1}{58060800}[\epsilon_4,[\epsilon_4,\epsilon_6]] + \tfrac{1}{47900160}[\epsilon_4^{(1)},\epsilon_{10}] - \tfrac{1}{383201280}[\epsilon_4,\epsilon_{10}^{(1)}] + \ldots \,.\end{aligned} \tag{5.46}$$

For $w=3$ it turns out that the key-degree part $\sigma_3^{\rm key}$ is already $\mathfrak{sl}_2$ invariant and therefore coincides with the arithmetic derivation z_3 whose action on a and b is given by

$$\begin{aligned} z_3(a) &= \tfrac{1}{4}[aaababb] + \tfrac{1}{4}[aaabbab] + \tfrac{1}{12}[aababab]\,, \\ z_3(b) &= -\tfrac{1}{4}[aababbb] - \tfrac{1}{4}[aabbabb] - \tfrac{1}{4}[aabbbab] - \tfrac{1}{12}[abababb]\,. \end{aligned} \tag{5.47}$$

An exact expression for the whole of the power series σ_3 will be given as a closed formula in section 7.4.3 below.

5.5.2 The case $w=5,7,9$

Now we give the lowest-degree contributions to the expansions of σ_5, σ_7 and σ_9:

$$\begin{aligned}\sigma_5 = &-\tfrac{1}{24}\epsilon_6^{(4)} - \tfrac{5}{48}[\epsilon_4^{(1)},\epsilon_4^{(2)}] + z_5 + \tfrac{1}{5760}[\epsilon_4,\epsilon_6^{(3)}] - \tfrac{1}{5760}[\epsilon_4^{(1)},\epsilon_6^{(2)}] + \tfrac{1}{5760}[\epsilon_4^{(2)},\epsilon_6^{(1)}] \\ &+ \tfrac{1}{3456}[\epsilon_4,[\epsilon_4,\epsilon_4^{(2)}]] + \tfrac{1}{6912}[\epsilon_4^{(1)},[\epsilon_4^{(1)},\epsilon_4]] + \tfrac{1}{145152}[\epsilon_6^{(1)},\epsilon_6^{(2)}] - \tfrac{1}{145152}[\epsilon_6,\epsilon_6^{(3)}] \\ &- \tfrac{1}{2073600}[\epsilon_4,[\epsilon_4,\epsilon_6^{(2)}]] + \tfrac{139}{72576000}[\epsilon_4^{(1)},[\epsilon_4,\epsilon_6^{(1)}]] - \tfrac{23}{24192000}[\epsilon_4,[\epsilon_4^{(1)},\epsilon_6^{(1)}]] \\ &- \tfrac{1007}{145152000}[\epsilon_4^{(2)},[\epsilon_4,\epsilon_6]] - \tfrac{1}{4147200}[\epsilon_4^{(1)},[\epsilon_4^{(1)},\epsilon_6]] + \tfrac{289}{48384000}[\epsilon_4,[\epsilon_4^{(2)},\epsilon_6]] \\ &+ \tfrac{1}{145152000}[\epsilon_6,\epsilon_8^{(3)}] - \tfrac{1}{36288000}[\epsilon_6^{(1)},\epsilon_8^{(2)}] + \tfrac{1}{14515200}[\epsilon_6^{(2)},\epsilon_8^{(1)}] - \tfrac{1}{7257600}[\epsilon_6^{(3)},\epsilon_8] + \ldots \end{aligned} \tag{5.48}$$

$$\begin{aligned}\sigma_7 = &-\tfrac{1}{720}\epsilon_8^{(6)} + \tfrac{7}{1152}[\epsilon_4^{(2)},\epsilon_6^{(3)}] - \tfrac{7}{1152}[\epsilon_4^{(1)},\epsilon_6^{(4)}] - \tfrac{661}{57600}[\epsilon_4^{(1)},[\epsilon_4^{(1)},\epsilon_4^{(2)}]] - \tfrac{661}{57600}[\epsilon_4^{(2)},[\epsilon_4^{(2)},\epsilon_4]] \\ &+ \tfrac{1}{172800}[\epsilon_4,\epsilon_8^{(5)}] - \tfrac{1}{172800}[\epsilon_4^{(1)},\epsilon_8^{(4)}] + \tfrac{1}{172800}[\epsilon_4^{(2)},\epsilon_8^{(3)}] + \tfrac{1}{13824}[\epsilon_6^{(1)},\epsilon_6^{(4)}] - \tfrac{1}{13824}[\epsilon_6^{(2)},\epsilon_6^{(3)}] \\ &+ z_7 - \tfrac{1}{4354560}[\epsilon_6,\epsilon_8^{(5)}] + \tfrac{1}{4354560}[\epsilon_6^{(1)},\epsilon_8^{(4)}] - \tfrac{1}{4354560}[\epsilon_6^{(2)},\epsilon_8^{(3)}] + \tfrac{1}{4354560}[\epsilon_6^{(3)},\epsilon_8^{(2)}] \\ &- \tfrac{1}{4354560}[\epsilon_6^{(4)},\epsilon_8^{(1)}] + \tfrac{7}{552960}[\epsilon_4,[\epsilon_4,\epsilon_6^{(4)}]] + \tfrac{7}{552960}[\epsilon_4,[\epsilon_4^{(1)},\epsilon_6^{(3)}]] + \tfrac{7}{184320}[\epsilon_4^{(1)},[\epsilon_4^{(2)},\epsilon_6^{(1)}]] \\ &+ \tfrac{7}{552960}[\epsilon_4^{(2)},[\epsilon_4,\epsilon_6^{(2)}]] - \tfrac{7}{184320}[\epsilon_4,[\epsilon_4^{(2)},\epsilon_6^{(2)}]] - \tfrac{7}{276480}[\epsilon_4^{(2)},[\epsilon_4^{(2)},\epsilon_6]] \\ &- \tfrac{7}{552960}[\epsilon_4^{(1)},[\epsilon_4,\epsilon_6^{(3)}]] - \tfrac{7}{552960}[\epsilon_4^{(2)},[\epsilon_4^{(1)},\epsilon_6^{(1)}]] + \ldots \end{aligned} \tag{5.49}$$

$$\begin{aligned}\sigma_9 = &-\tfrac{1}{40320}\epsilon_{10}^{(8)} - \tfrac{1}{5184}[\epsilon_4^{(1)},\epsilon_8^{(6)}] + \tfrac{1}{5184}[\epsilon_4^{(2)},\epsilon_8^{(5)}] - \tfrac{7}{20736}[\epsilon_6^{(3)},\epsilon_6^{(4)}] + \tfrac{1}{9676800}[\epsilon_4,\epsilon_{10}^{(7)}] \\ &- \tfrac{1}{9676800}[\epsilon_4^{(1)},\epsilon_{10}^{(6)}] + \tfrac{1}{9676800}[\epsilon_4^{(2)},\epsilon_{10}^{(5)}] + \tfrac{7}{4147200}[\epsilon_6^{(1)},\epsilon_8^{(6)}] - \tfrac{7}{4147200}[\epsilon_6^{(2)},\epsilon_8^{(5)}] \\ &+ \tfrac{7}{4147200}[\epsilon_6^{(3)},\epsilon_8^{(4)}] - \tfrac{7}{4147200}[\epsilon_6^{(4)},\epsilon_8^{(3)}] - \tfrac{529}{691200}[\epsilon_4,[\epsilon_4^{(2)},\epsilon_6^{(4)}]] + \tfrac{2959}{2419200}[\epsilon_4^{(1)},[\epsilon_4^{(2)},\epsilon_6^{(3)}]] \\ &+ \tfrac{5891}{6220800}[\epsilon_4^{(2)},[\epsilon_4,\epsilon_6^{(4)}]] - \tfrac{443}{967680}[\epsilon_4^{(1)},[\epsilon_4^{(1)},\epsilon_6^{(4)}]] - \tfrac{799}{1088640}[\epsilon_4^{(2)},[\epsilon_4^{(2)},\epsilon_6^{(2)}]] \\ &- \tfrac{10651}{21772800}[\epsilon_4^{(2)},[\epsilon_4^{(1)},\epsilon_6^{(3)}]] + \ldots \end{aligned} \tag{5.50}$$

In all cases, the ellipsis refers to an infinite series in nested brackets of $\epsilon_{k_i}^{(j_i)}$ of total degree $\sum_i k_i \geq 16$, and the expansion of σ_9 additionally involves an arithmetic contribution z_9 at key degree 18. The action of the arithmetic derivation z_5 on the generators a is given by

$$\begin{aligned} z_5(a) = &-\frac{[aaaaababbbb]}{240} - \frac{[aaaaabbbbab]}{240} + \frac{[aaaabaabbbb]}{120} + \frac{[aaaabababbb]}{80} - \frac{[aaaababbabb]}{30} \\ &+ \frac{[aaaababbbab]}{60} + \frac{[aaaabbaabbb]}{80} - \frac{7[aaaabbababb]}{120} - \frac{[aaaabbabbab]}{30} + \frac{[aaaabbbaabb]}{80} \\ &+ \frac{[aaaabbbabab]}{240} + \frac{[aaaabbbbaab]}{240} - \frac{[aaabaababbb]}{24} - \frac{3[aaabaabbabb]}{80} - \frac{7[aaabaabbbab]}{240} \\ &- \frac{[aaababaabbb]}{240} + \frac{73[aaabababababb]}{240} + \frac{49[aaabababbab]}{80} + \frac{3[aaababbaabb]}{80} + \frac{149[aaababbabab]}{240} \\ &+ \frac{[aaababbbaab]}{240} - \frac{[aaabbaababb]}{240} - \frac{[aaabbaabbab]}{60} + \frac{[aaabbabaabb]}{240} + \frac{5[aaabbababab]}{16} \\ &- \frac{[aaabbabbaab]}{240} + \frac{[aaabbbaabab]}{240} + \frac{[aaabbbabaab]}{120} + \frac{[aabaabaabbb]}{240} + \frac{[aabaabababb]}{240} \\ &- \frac{[aabaababbab]}{30} + \frac{[aabaabbaabb]}{120} - \frac{[aabaabbabab]}{30} - \frac{3[aababaababb]}{80} - \frac{3[aababaabbab]}{80} \\ &- \frac{[aabababaabb]}{240} + \frac{[aababababab]}{16}\,, \end{aligned} \tag{5.51}$$

again using the Lyndon bracket notation of Theorem 3.5.2. A similar expression for $z_5(b)$ can be reconstructed from (5.51) by virtue of the following observation:

Remark 5.5.1. The Lie polynomials $z_w(a)$ and $z_w(b)$ at $w = 3$, $w = 5$ and $w = 7$ are related by the switch θ via

$$z_w(b) = -\theta\big(z_w(a)\big)\,, \qquad w \leq 7\,. \tag{5.52}$$

Note that an alternative method for the computation of $z_3(a), z_3(b), z_5(a), z_5(b)$ was given by Pollack in [26], though the approach in that reference has not yet led to explicit results for $z_{w\geq 7}$. Machine-readable expressions for $z_w(a)$ and $z_w(b)$ at $w = 3, 5, 7$ can be found in an ancillary file of the arXiv submission of this work.

5.5.3 Computational aspects

We close this section by giving more details on the practical implementation of Definition 5.2.3 to determine the canonical zeta generators σ_w and their arithmetic parts z_w.

The starting point of the construction is to solve the conditions (5.41) degree by degree following (5.36) and (5.37) and the partner condition. We recall from Theorem 5.4.1 that at degree d the derivation $(\sigma_w)_d$ has a-degree $d-w$ and b-degree w.

For the example of σ_3 the extension lemma leads at lowest degree to[9]

$$\big(\sigma_3(a)\big)_5 = -[aabbb] + [ababb]\,, \quad \big(\sigma_3(b)\big)_5 = -[abbbb]\,, \tag{5.53}$$

by using g_3 presented in (3.32) as well as (5.36). We here employ Lyndon bracket notation in the Lie algebra Lie$[a, b]$. From (5.37) we then obtain at the next degree (which is here already key degree):

$$\begin{aligned} \big(\sigma_3(a)\big)_7 &= \tfrac{1}{4}[aaababb] + \tfrac{1}{4}[aaabbab] + \tfrac{1}{12}[aababab]\,, \\ \big(\sigma_3(b)\big)_7 &= -\tfrac{1}{4}[aababbb] - \tfrac{1}{4}[aabbabb] - \tfrac{1}{4}[aabbbab] - \tfrac{1}{12}[ababab b]\,. \end{aligned} \tag{5.54}$$

[9]Note that, as a derivation, the lowest degree of σ_3 is 4, but here we are writing the degree of the image of a and b as the subscript.

Since (5.53) is not at key degree, we know from Theorem 5.4.1 that it must be possible to rewrite it completely as the action of a geometric derivation, i.e. an element of $\mathfrak{u}$. We know moreover from part (ii) of that theorem that the *total depth*, meaning the total number of ϵ_i (for $i \geq 0$) of any term is equal to $w = 3$. Together with the information on the degree, computable from Lemma 5.1.5, this leaves very few possible terms. For any nested backet of the form $\epsilon_{k_1}^{(j_1)} \cdots \epsilon_{k_r}^{(j_r)}$ (with $k_i \geq 4$ and any allowed placement of brackets) the conditions to be allowed at degree d in σ_w are

$$
\begin{aligned}
r + \sum_{i=1}^{r} j_i &= w && \text{for the total depth and} \\
\sum_{i=1}^{r} k_i &= d && \text{for the degree.}
\end{aligned}
\tag{5.55}
$$

For example, for the lowest degree $d = 4$ in (5.53), the only possible term in σ_3 is proportional to $\epsilon_4^{(2)}$ and the constant of proportionality c_1 is fixed by

$$\big(\sigma_3(a)\big)_5 = \Big[\big(c_1\epsilon_4^{(2)}\big)(a)\Big]_5 = c_1\,(2[aabbb] - 2[ababb]) \tag{5.56}$$

to the value $c_1 = -\frac{1}{2}$ when comparing to (5.53), in agreement with (5.46) and a general formula to be derived in Corollary 6.2.3.

The next-to-lowest degree in σ_3, given by (5.54), is the key degree $d = 2w = 6$ and therefore contains both the arithmetic z_3 part, transforming in an $\mathfrak{sl}_2$ singlet, as well as possible geometric contributions. The most general ansatz compatible with (5.55) is

$$\sigma_3^{\text{key}} = z_3 + c_2\epsilon_6^{(2)}\,. \tag{5.57}$$

In order to separate out the geometric from the arithmetic term, we use that z_3 is a singlet under $\mathfrak{sl}_2$ and thus commutes with ϵ_0. The general relations

$$\epsilon_0\big(\sigma_w(a)\big) - \sigma_w(b) = [\epsilon_0, \sigma_w](a)\,, \qquad \epsilon_0\big(\sigma_w(b)\big) = [\epsilon_0, \sigma_w](b) \tag{5.58}$$

at key degree depend only on the geometric part due to $[\epsilon_0, \sigma_w^{\text{key}}] = [\epsilon_0, \sigma_w^{\text{key}} - z_w]$. Moreover, the commutator $[\epsilon_0, \sigma_w^{\text{key}} - z_w]$ of the geometric term can be evaluated easily according to general representation theory as in Lemma 5.1.5. The left-hand sides of the general conditions (5.58) only depend on $\sigma_w(a)$ and $\sigma_w(b)$ that are furnished by (5.41) whereas the geometric contribution on the right-hand sides can be computed using the ansatz.

In the case of (5.54) we can use the second equation of (5.58) and find for the left-hand side

$$\epsilon_0\big(\sigma_3^{\text{key}}(b)\big) = 0 \tag{5.59}$$

as well as

$$c_2\epsilon_6^{(3)}(b) = 12c_2\big(2[aabbbb] + 5[ababbbb] + 2[abbabbb]\big) \tag{5.60}$$

for the right-hand side, implying $c_2 = 0$ and that the action of z_3 is given by (5.54), which agrees with the expression already presented in (5.47).

The ansätze for the degree d parts of σ_w rapidly grow with d and w. For instance, the candidate terms for $(\sigma_7)_{12}$ compatible with (5.55) are given by

$$
\begin{aligned}
(\sigma_7)_{12} = c_1\epsilon_{12}^{(6)} + c_2[\epsilon_4, \epsilon_8^{(5)}] + c_3[\epsilon_4^{(1)}, \epsilon_8^{(4)}] + c_4[\epsilon_4^{(2)}, \epsilon_8^{(3)}] \\
+ c_5[\epsilon_6^{(1)}, \epsilon_6^{(4)}] + c_6[\epsilon_6^{(2)}, \epsilon_6^{(3)}] + c_7[\epsilon_4^{(1)}, [\epsilon_4^{(1)}, \epsilon_4^{(2)}]] + c_8[\epsilon_4^{(2)}, [\epsilon_4^{(2)}, \epsilon_4]] \, .
\end{aligned}
\tag{5.61}
$$

By matching the action of this ansatz on a with $\big(\sigma_7(a)\big)_{13}$ computed from (5.41), we find the values of the above c_i noted in the degree 12 parts of (5.49) including a vanishing coefficient c_1 of $\epsilon_{12}^{(6)}$. The absence of terms in σ_w with a single $\epsilon_k^{(j)}$ at any degree besides the minimal degree $w+1$ will follow from Proposition 7.3.4 (i) below.

In summary, the strategy for converting the result of the extension lemma construction of σ_w into expressions in terms of geometric and arithmetic derivations is to make an ansatz for the geometric terms at a given degree subject to the constraints (5.55).[10] Away from key degree, evaluating this ansatz on a and b and equating it with the explicit form of σ_w then fixes the ansatz (modulo free parameters that are in one-to-one correspondence with the Pollack relations defining $\mathfrak{u}$). At key degree one can separate the geometric from the arithmetic part of σ_w using (5.58) by first computing the geometric part; then the arithmetic z_w is simply the difference $z_w = \sigma_w^{\rm key} - \big(\sigma_w^{\rm key}|_{\mathfrak{u}}\big)$.

In section 7.3, we will provide additional calculational tools that recursively determine σ_w up to highest-weight vectors of $\mathfrak{sl}_2$ (see Definition 5.1.3). In case of (5.61), the ansatz contains two highest-weight vectors $[\epsilon_6^{(1)}, \epsilon_6^{(4)}] - [\epsilon_6^{(2)}, \epsilon_6^{(3)}]$ and $[\epsilon_4^{(1)}, [\epsilon_4^{(1)}, \epsilon_4^{(2)}]] + [\epsilon_4^{(2)}, [\epsilon_4^{(2)}, \epsilon_4]]$, and the method of section 7.3 can efficiently determine 6 out of the 8 parameters c_i. By Theorem 5.4.1 (iv), there are no highest-weight vectors in σ_w beyond key degree. Hence, a major virtue of the method in 7.3 is that the evaluation of *infinitely* many contributions $\sigma_w(a)_{d>2w+1}$ via (5.41) can be bypassed, i.e. that the extension lemma construction of section 5.3 only needs to be applied to a *finite* range of degrees where it fixes *all* terms.

6 Properties of τ_w and σ_w

In this section, we prove the properties of the derivation τ_w, σ_w or zeta generators in genus one listed in Theorem 5.4.1 (i) to (vi). One of the key tools for parts (i)-(iii) will be Écalle's theory of moulds developed in [22] (see also [80] for an exposition of the basic theory), and the proof of parts (iv)-(vi) will make use of the $\mathfrak{sl}_2$ algebra in Definition 5.1.3.

6.1 Introduction to moulds

For the reader's convenience, we first review a few basic definitions and facts about moulds, and one fundamental theorem due to Écalle (cf. [22], [80]).

[10] It can be useful, although not necessary, to group these terms according to $\mathfrak{sl}_2$ representations.

6.1.1 Moulds and power series

Definition 6.1.1. A *rational mould* over a ring R is a family of rational functions $F = \big(F_r\big)_{r\geq 0} = (F_0, F_1, F_2, \ldots)$ such that

$$F_r(u_1, \ldots, u_r) \in R(u_1, \ldots, u_r)\,, \tag{6.1}$$

i.e. F_r is a function of r commutative variables u_i. The *constant term* of the mould F_0 lies in the ring R. We will generally refer to a rational mould simply as a "mould", and most of the time we will work over the base field $\mathbb{Q}$. Also, when there is no possibility of confusion, we often write $F(u_1, \ldots, u_r)$ instead of $F_r(u_1, \ldots, u_r)$. The function F_r or $F(u_1, \ldots, u_r)$ is called the *depth r part of the mould F*. When the rational functions F_r are polynomials for all $r > 0$, we say that F is a *polynomial mould*. Moulds can be added componentwise and multiplied by a constant in R componentwise. The moulds with constant term 0 thus form a vector space, denoted ARI; its vector subspace of polynomial moulds is denoted ARI^{pol}. The names of the various objects, morphisms and properties are due to Écalle [22].

Let $c_i = \mathrm{ad}_x^{i-1} y$ for $i \geq 1$. From now on unless otherwise stated we will work with $R = \mathbb{Q}$. The power series in $\mathbb{Q}\langle\langle x, y\rangle\rangle$ that can be written as power series in the c_i are exactly the ring of power series p satisfying $\partial_x(p) = 0$, where ∂_x is the derivation defined by $\partial_x(x) = 1$, $\partial_x(y) = 0$. These power series are in bijection with the free ring $\mathbb{Q}\langle\langle c_1, c_2, \ldots\rangle\rangle$ of power series on the non-commutative variables c_i. All Lie-like and group-like power series in $\mathbb{Q}\langle\langle x, y\rangle\rangle$ belong to $\mathbb{Q}\langle\langle c_1, c_2, \ldots\rangle\rangle$ and indeed, with the exception of the element x, all Lie polynomials in x, y are in bijection with the Lie polynomials in the c_i. There is a simple bijection between power series $p \in \mathbb{Q}\langle\langle c_1, c_2, \ldots\rangle\rangle$ and polynomial moulds, given by letting p^r denote the part of p of homogeneous degree r in the c_i (i.e. homogeneous degree r in y) and mapping p^r to the space of polynomial moulds of depth r by the map on monomials

$$ma : c_{i_1} \ldots c_{i_r} \mapsto (-1)^{r+i_1+\cdots+i_r} u_1^{i_1-1} \cdots u_r^{i_r-1}\,, \tag{6.2}$$

extended by linearity. We often use the notation $P = ma(p)$ for the polynomial mould associated to a power series $p \in \mathbb{Q}\langle\langle c_1, c_2, \ldots\rangle\rangle$ under the map ma. The vector space of power series without constant term maps isomorphically under ma to the vector space ARI^{pol}.

6.1.2 Basic operators on moulds

The space of moulds ARI is equipped with many operations. All those given in the following list are natural extensions to moulds of familiar operations on power series in x and y (see [22] or [80] for complete definitions and details).

- Mould multiplication is defined by:

$$mu(G, H)(u_1, \ldots, u_r) = \sum_{i=0}^{r} G(u_1, \ldots, u_i) H(u_{i+1}, \ldots, u_r)\,. \tag{6.3}$$

This multiplication is valid for moulds with non-zero constant term as well, and is compatible with power series multiplication in the sense that if $G = ma(g)$ and $H = ma(h)$ for $g, h \in \mathbb{Q}\langle\langle c_1, c_2, \ldots, \rangle\rangle$, then

$$ma\big(gh\big) = mu(G, H)\,. \tag{6.4}$$

- The Lie bracket lu on ARI is defined by

$$lu(G, H) = mu(G, H) - mu(H, G)\,, \tag{6.5}$$

and when ARI is considered as a Lie algebra under this bracket, it is denoted ARI_{lu}. Again, for $G = ma(g)$ and $H = ma(h)$ as above, we have

$$ma\big([g, h]\big) = lu(G, H)\,. \tag{6.6}$$

- For each mould $G \in ARI$, there is a derivation $arit(G)$ of the Lie algebra ARI_{lu} which generalizes the Ihara derivation D_g for $g \in \mathrm{Lie}[x, y]$ defined by (3.15) in the sense that if $G = ma(g)$ and $H = ma(h)$ for $g, h \in \mathrm{Lie}[x, y]$ then

$$arit(G) \cdot H = -ma\big(D_g(h)\big)\,. \tag{6.7}$$

(The minus sign is due to the original definition of *arit* by Écalle).

- The *ari-bracket* is another Lie bracket on the space ARI (besides lu introduced in (6.5)), defined by

$$ari(G, H) = arit(H) \cdot G - arit(G) \cdot H + lu(G, H)\,. \tag{6.8}$$

The ari-bracket generalizes the Ihara bracket (3.14) on the underlying vector space $\mathrm{Lie}[x, y]$ in the sense that if $G = ma(g)$ and $H = ma(h)$ for $g, h \in \mathrm{Lie}[x, y]$ then

$$ari(G, H) = ma\big(\{g, h\}\big)\,. \tag{6.9}$$

We denote the Lie algebra formed by the vector space ARI equipped with the *ari*-bracket by ARI_{ari}.

- The universal enveloping algebra $\mathcal{U}ARI_{ari}$ of the Lie algebra ARI_{ari} is nothing other than the space of all (rational in the context of this article) moulds; these are essentially the same moulds as in ARI except that arbitrary constant terms are allowed. By the Poincaré–Birkhoff–Witt theorem, this universal enveloping algebra is equipped with an associative multiplication law which we denote by $\diamond$. The expression for this multiplication $G \diamond H$ simplifies in the case where $G \in ARI$, in which situation it is given for G in ARI_{ari} and H in $\mathcal{U}ARI_{ari}$ by

$$G \diamond H = mu(G, H) - arit(G) \cdot H\,, \tag{6.10}$$

which thanks to (6.7) generalizes the $\diamond$ multiplication introduced in (3.17):

$$G \diamond H = ma\big(g \diamond h\big). \tag{6.11}$$

- The *ari-exponential* map from ARI_{ari} to the group-like elements in the universal enveloping algebra is defined for $F \in ARI$ by

$$\exp_{ari}(F) = Id + \sum_{n\geq 1} \frac{1}{n!}\big(\underbrace{F \diamond F \diamond \ldots \diamond F}_{n}\big)\,, \tag{6.12}$$

where the $\diamond$ multiplication must be applied from right to left so that the leftmost element being multiplied is always F, and Id denotes the *mu*- and $\diamond$-identity mould $(1, 0, 0, \ldots)$. The image of the space ARI under the map $\exp_{ari}$ is called $GARI$, and it consists precisely of the set of all (here rational) moulds with constant term 1. The set $GARI$ forms a group with respect to the multiplication obtained from lifting the *ari* Lie bracket to $GARI$ using the Baker–Campbell–Hausdorff formula. The ari-exponential has an inverse map, the *ari-logarithm*

$$\log_{ari} : GARI \to ARI\,. \tag{6.13}$$

- The group $GARI$ acts on the Lie algebra ARI_{ari} via the *adjoint action*, under which each mould $P \in GARI$ gives an isomorphism of the Lie algebra ARI_{ari} via the *adjoint operator* $\mathrm{Ad}_{ari}(P)$. Let $L := \log_{ari}(P)$, so $L \in ARI$. Then the adjoint action of P on a mould $A \in ARI$ can be expressed and computed explicitly by the standard formula

$$\mathrm{Ad}_{ari}(P)(A) = A + ari(L, A) + \tfrac{1}{2}ari(L, ari(L, A)) + \tfrac{1}{6}ari(L, ari(L, ari(L, A))) + \cdots \tag{6.14}$$

by exponentiating the *ari* bracket $ari(L, \cdot)$.

- We define an operator *dur* acting on all moulds by $dur(F)(\emptyset) = F(\emptyset)$ and the following formula for $r \geq 1$:

$$dur(F)(u_1, \ldots, u_r) = (u_1 + \cdots + u_r)F(u_1, \ldots, u_r)\,. \tag{6.15}$$

If $F = ma(f)$ for a power series $f \in \mathbb{Q}\langle\langle c_1, c_2, \ldots\rangle\rangle$ (considered as a function $f(x, y)$), then

$$dur(F) = ma([x, f])\,. \tag{6.16}$$

- We will also need the mould operator Δ defined by $\Delta(F)(\emptyset) = F(\emptyset)$ and

$$\Delta(F)(u_1, \ldots, u_r) = u_1 \cdots u_r(u_1 + \cdots + u_r)F(u_1, \ldots, u_r)\,. \tag{6.17}$$

If $F = ma(f)$ as above, we have

$$\Delta(F) = ma\big([x, f(x, [x, y])]\big)\,. \tag{6.18}$$

The inverse operator of Δ is given by

$$\Delta^{-1}(F)(u_1, \ldots, u_r) = \frac{1}{u_1 \cdots u_r(u_1 + \cdots + u_r)}F(u_1, \ldots, u_r)\,. \tag{6.19}$$

Of course, the operator Δ on power series given in (6.18) cannot always be inverted in the world of non-commutative power series.

- The *push-operator* acts on moulds F by the formula $push(F)(\emptyset) = F(\emptyset)$ and for $r \geq 1$,

$$push(F)(u_1, \dots, u_r) = F(-u_1 - \cdots - u_r, u_1, u_2, \dots, u_{r-1})\,. \tag{6.20}$$

  The push-operator corresponds to an operation on power series (also called push) monomial by monomial defined as follows:

$$push(x^{a_1} y x^{a_2} y \cdots y x^{a_r-1} y x^{a_r}) = x^{a_r} y x^{a_1} y \cdots y x^{a_r-2} y x^{a_{r-1}} \tag{6.21}$$

  in the sense that if $h \in \mathbb{Q}\langle\langle c_1, c_2, \dots \rangle\rangle$ then

$$ma\big(push(h)\big) = push\big(ma(h)\big)\,, \tag{6.22}$$

  where the left-hand push is as in (6.21) and the right-hand one is as in (6.20) (for this equivalence, see [81], section 3.3). In particular, h is push-invariant if and only if $ma(h)$ is.

- The *swap* operator on moulds is defined by the formula $swap(F)(\emptyset) = F(\emptyset)$ and

$$swap(F)(v_1, v_2, \dots, v_r) = F(v_r, v_{r-1} - v_r, \dots, v_1 - v_2)\,. \tag{6.23}$$

  We could write the mould $swap(F)$ in the variables u_i instead of v_i, of course, but to keep apart a mould and its swap it is convenient to consider the swapped mould parts $swap(F)_r$ as lying in $\mathbb{Q}(v_1, \dots, v_r)$.

- Finally, we need to define the *alternality* property on moulds. A mould $P \in ARI$ is said to be *alternal* if for all $r \geq 2$ we have

$$\sum_{w \in u \sqcup\!\sqcup v} P(w) = 0 \tag{6.24}$$

  for all pairs of non-empty words $u = (u_1, \dots, u_i)$, $v = (u_{i+1}, \dots, u_r)$. (There is no condition at $r = 1$.) When $P = ma(p)$ for a power series $p \in \mathbb{Q}\langle\langle c_1, c_2, \dots \rangle\rangle$ without constant term, then P is alternal if and only if p is a Lie element in the c_i, or equivalently, if and only if $p(x, y) \in \mathrm{Lie}[x, y]$.

Example. Recall that the first non-trivial element of $\mathfrak{mz}^\vee$ is given by

$$g_3 = [x, [x, y]] + [[x, y], y] = c_3 + [c_2, c_1] = c_3 + c_2 c_1 - c_1 c_2\,. \tag{6.25}$$

By (6.2), the associated mould $G_3 = ma(g_3) \in ARI$ is given by

$$\begin{aligned} 0 &\mapsto 0 = G_3(\emptyset) && \text{in depth } 0\,, \\ c_3 &\mapsto u_1^2 = G_3(u_1) && \text{in depth } 1\,, \\ c_2 c_1 - c_1 c_2 &\mapsto -u_1 + u_2 = G_3(u_1, u_2) && \text{in depth } 2\,. \end{aligned} \tag{6.26}$$

The fact that g_3 is a Lie polynomial is reflected in the alternality condition satisfied by G_3:

$$\sum_{w \in (u_1 \sqcup\!\sqcup u_2)} G_3(w) = G_3(u_1, u_2) + G_3(u_2, u_1) = 0\,. \tag{6.27}$$

6.1.3 The fundamental operator $\mathrm{Ad}_{ari}(pal)$ and Écalle's theorem

Écalle defined a remarkable pair of inverse moulds in the group $GARI$, called pal and $invpal$, which have the following property: when acting on ARI via the adjoint action, $invpal$ transforms the double shuffle property into a much simpler property known as *bialternality*, where a bialternal mould is an alternal mould with alternal swap, and pal does the opposite (this is a major result due to Écalle, see [22, 82] and an expository version in section 4.6 of [80]). The isomorphisms $\mathrm{Ad}_{ari}(invpal)$ and $\mathrm{Ad}_{ari}(pal)^{-1}$ are mutually inverse. The action of $\mathrm{Ad}_{ari}(invpal)$ on a double shuffle Lie polynomial mould introduces certain denominators, but these are eliminated by the operator Δ in (6.17), yielding a polynomial mould once again (cf. [83]); in other words, restricted to $ma(\mathfrak{ds})$, the composition $\Delta\circ\mathrm{Ad}_{ari}(invpal)$ takes polynomial moulds to polynomial moulds. The key result for our purposes here is that when restricted to the subspace $ma(\mathfrak{mz}^\vee)\subset ma(\mathfrak{ds})$, the map $\Delta\circ\mathrm{Ad}_{ari}(invpal)$ is directly related to the morphism

$$\gamma:\mathfrak{mz}^\vee\to \mathrm{Der}^0\mathrm{Lie}[a,b] \tag{6.28}$$

of (5.26) by the following formula: if $h\in\mathfrak{mz}^\vee$, then

$$\Delta\circ\mathrm{Ad}_{ari}(invpal)\big(ma(h)\big)=ma\big(\gamma(h)(a)\big)\,, \tag{6.29}$$

where

$$\gamma(h)\in\mathrm{Der}^0\mathrm{Lie}[a,b] \tag{6.30}$$

and $\gamma(h)(a)$ denotes the Lie series obtained by applying that derivation to a (cf. [23], Thm. 1.3.1). The connection (6.29) enables us to apply the known properties of the operator $\mathrm{Ad}_{ari}(invpal)$ to prove properties of the derivations τ_w and σ_w.

We now proceed to the definition of the moulds pal and $invpal$.

Definition 6.1.2. Let $dupal$ be the mould defined explicitly by $dupal(\emptyset)=0$ and for $r>0$ by

$$dupal(u_1,\ldots,u_r)=\frac{\mathrm{B}_r}{r!}\frac{1}{u_1\cdots u_r}\left(\sum_{j=0}^{r-1}(-1)^j\binom{r-1}{j}u_{j+1}\right). \tag{6.31}$$

Lemma 6.1.3. *The mould dupal is related to t_{01} in (5.30) by the equation*

$$dupal(u_1,\ldots,u_r)=\frac{1}{u_1\cdots u_r}ma(t_{01}^r) \tag{6.32}$$

for all $r\geq 1$, where t_{01}^r is the part of t_{01} of b-degree r.

Proof. The map ma maps power series in a,b to moulds exactly like those in x,y, namely via (6.2) with $c_i=\mathrm{ad}_a^{i-1}(b)$. To prove (6.32), notice that since we have

$$\mathrm{ad}_b^{r-1}(a)=-\mathrm{ad}_b^{r-2}([a,b])=-\mathrm{ad}_{c_1}^{r-1}(c_2)=-\sum_{j=0}^{r-1}(-1)^j\binom{r-1}{j}c_1^jc_2c_1^{r-1-j}\,, \tag{6.33}$$

the associated mould is

$$ma\big(\mathrm{ad}_b^{r-1}(a)\big) = -\sum_{j=0}^{r-1}(-1)^j\binom{r-1}{j}u_{j+1}\,. \tag{6.34}$$

Hence, since the part t_{01}^r of b-degree r of t_{01} is just given by $-\frac{\mathrm{B}_r}{r!}\mathrm{ad}_b^r(a)$, (6.32) follows from comparing (6.31) and (6.34). □

Definition 6.1.4. Let *pal* be the mould defined recursively by $pal(\emptyset) = 1$ and the formula

$$dur(pal) = mu(pal, dupal) \tag{6.35}$$

with *dur* defined in (6.15) and *dupal* in (6.31).

This formula might look circular but in fact it defines each depth of *pal* successively thanks to the fact that $dupal(\emptyset) = 0$. For example, in depth 1, we have

$$\begin{aligned} dur(pal)(u_1) &= u_1 pal(u_1) \\ &= mu(pal, dupal)(u_1) \\ &= pal(\emptyset)dupal(u_1) + pal(u_1)dupal(\emptyset) \\ &= dupal(u_1) \\ &= -\frac{1}{2}\,, \end{aligned} \tag{6.36}$$

so

$$pal(u_1) = -\frac{1}{2u_1}\,. \tag{6.37}$$

Then in depth 2, we have

$$\begin{aligned} dur(pal)(u_1, u_2) &= (u_1 + u_2)pal(u_1, u_2) \\ &= mu(pal, dupal)(u_1, u_2) \\ &= pal(\emptyset)dupal(u_1, u_2) + pal(u_1)dupal(u_2) \\ &= \frac{u_1 - u_2}{12u_1u_2} + \frac{1}{4u_1} \\ &= \frac{u_1 + 2u_2}{12u_1u_2}\,, \end{aligned} \tag{6.38}$$

so

$$pal(u_1, u_2) = \frac{u_1 + 2u_2}{12u_1u_2(u_1 + u_2)}\,. \tag{6.39}$$

Definition 6.1.5. Let $lopal = \log_{ari}(pal)$ using the ari-logarithm map defined in (6.13), and recall that *invpal* is the inverse of *pal* in the group $GARI = \exp_{ari}(ARI)$, equipped with the Baker–Campbell–Hausdorff multiplication law, so that we have

$$\log_{ari}(pal) = -\log_{ari}(invpal)\,. \tag{6.40}$$

In lowest depths we have

$$\begin{aligned} lopal &= \left(0,\ -\frac{1}{2u_1},\ \frac{u_1-u_2}{12u_1u_2(u_1+u_2)},\ \dots\right), \\ invpal &= \left(1,\ \frac{1}{2u_1},\ \frac{-u_1+4u_2}{12u_1u_2(u_1+u_2)},\ \dots\right). \end{aligned} \tag{6.41}$$

Both of these moulds will be used below in our computations of σ_w.

The following theorem summarizes the key results from mould theory needed for the proof of Theorem 5.4.1 (i) to (iii).

Theorem 6.1.6. *Let $h \in \mathfrak{ds}$ and let $H = ma(h)$ denote the associated mould. Let τ_h be the derivation of $\widehat{\mathrm{Lie}}[a,b]$ constructed from h as in section 5.3 and write $T_h = ma\big(\tau_h(a)\big)$. Then,*

(i) The mould $\mathrm{Ad}_{ari}(invpal)(H)$ is bialternal, i.e. it is alternal and its swap is alternal (cf. [22, 82] and [80], Thm. 4.6.1);

(ii) We have the following equality of moulds in ARI (cf. [23], Thm. 1.3.1):

$$T_h = \Delta \circ \mathrm{Ad}_{ari}(invpal)(H)\,; \tag{6.42}$$

(iii) All bialternal moulds are push-invariant (cf. [22], [80] Lemma 2.5.5); in particular $\mathrm{Ad}_{ari}(invpal)(H)$ is push-invariant, and so is T_h since Δ does not modify push-invariance;

(iv) A bialternal rational mould A satisfies

$$A(-u_1, \dots, -u_r) = A(u_1, \dots, u_r) \tag{6.43}$$

for all $r \geq 1$. In particular if $A(u_1, \dots, u_r)$ is of odd total degree then it is equal to zero (cf. [80], Lemma 2.5.5).

Note that the push invariance of T_h and therefore $\tau_h(a)$ established in part (iii) is crucial to obtain extensions of derivations of the Lie subalgebra $\mathrm{Lie}[t_{12}, t_{01}] \subset \widehat{\mathrm{Lie}}[a,b]$ to all of $\mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$, see the discussion around (5.37).

6.2 Proof of Theorem 5.4.1 (i)-(iii)

For all $h \in \mathfrak{mz}^\vee$, let τ_h denote the associated derivation in $\mathrm{Der}^0\mathrm{Lie}[a,b]$ constructed in section 5.3. Let g_w for odd $w \geq 3$ be the canonical free generators of $\mathfrak{mz}^\vee$; recall that we write τ_w and σ_w for the zeta generators in genus one rather than τ_{g_w} and σ_{g_w}. The results of Theorem 6.1.6 are valid for all elements $h \in \mathfrak{ds}$, in particular for elements of the subspace $\mathfrak{mz}^\vee \subset \mathfrak{ds}$, but in this section we will apply them specifically to the elements g_w.

Corollary 6.2.1 (Theorem 5.4.1 (i)). *The derivations τ_w and σ_w satisfy*

$$\tau_w([a,b]) = \sigma_w([a,b]) = 0\,, \tag{6.44}$$

i.e. τ_w and σ_w lie in $\mathrm{Der}^0\mathrm{Lie}[a,b]$.

Proof. The mould $T_w = ma\big(\tau_w(a)\big)$ is push-invariant by Theorem 6.1.6 (iii), and we saw in (6.22) that push-invariance for moulds is equivalent to push-invariance of power series. Thus $\tau_w(a)$ is push-invariant. It is shown in Lemma 2.1.1 of [23] that for any derivation δ of $\mathrm{Lie}[a,b]$ such that $\delta(b)$ is the partner of $\delta(a)$ as defined in (5.31), then $\delta([a,b]) = 0$ if and only if $\delta(a)$ is push-invariant. Since $\tau_w(b)$ is the partner of $\tau_w(a)$ by construction (i.e. (5.31) with $g = \tau_w(a)$ and $g' = \tau_w(b)$) and $\tau_w(a)$ is push-invariant, we thus have $\tau_w([a,b]) = 0$ as desired. Then

$$\sigma_w([a,b]) = \theta \circ \tau_w \circ \theta([a,b]) = \theta \circ \tau_w([b,a]) = 0 \tag{6.45}$$

as well. □

Proposition 6.2.2. *The mould T_w is zero in all even depths, and in odd depths $r \geq 1$, $T_w(u_1,\ldots,u_r)$ is a polynomial of homogeneous degree $w+1$ in the variables u_i. In particular*

$$T_w(u_1) = u_1^{w+1}\,. \tag{6.46}$$

Proof. We first show that the mould T_w is of constant degree $w+1$ in $u_1,\ldots,u_r$ in every depth. For this, we begin by noting that the Lie series

$$\tau_w(t_{01}) = [t_{01}, g_w(t_{12}, -t_{01})] \tag{6.47}$$

has constant a-degree equal to $w+1$ since g_w is a polynomial of homogeneous degree w and both t_{01} and t_{12} have a-degree 1. Then, using the degree-by-degree computation of $\tau_w(a)$ given in (5.34) to (5.37) (with $h = g_w$), we see that $\tau_w(a)_n$ is a Lie polynomial of constant a-degree $w+1$ in every degree n since the a-degree of the partner $\tau_w(b)$ is one less than that of $\tau_w(a)$ at every degree. By the defining property $g_w(x,y)|_{x^{w-1}y} = 1$ of the canonical polynomials in genus zero and their symmetry property $g_w(x,y) = g_w(y,x)$,[11] the monomial $y^{w-1}x$ also appears in $g_w(x,y)$ with coefficient 1. Since $g_w(x,y)$ for odd w is a Lie polynomial this implies that the Lie word $ad(y)^{w-1}(x)$ appears in g_w with coefficient 1. Thus the minimal x-degree in g_w is 1 and by (5.36) we have

$$\tau_w(a)_{w+2} = [a, \mathrm{ad}_a^{w-1}([a,b])] = \mathrm{ad}_a^{w+1}(b)\,, \tag{6.48}$$

where the sign disappears since w is odd.

Under the map ma from power series to commutative variables $u_1,\ldots,u_r$ defined in (6.2) (with $c_i = \mathrm{ad}_a^{i-1}b$ for $i \geq 1$), we see that the a-degree corresponds to the degree in $u_1,\ldots,u_r$

[11] This symmetry property follows from the odd degree w of g_w together with the facts that $g_w(x,-y) \in \mathfrak{grt}$ by (5.24) and that one of the defining properties of elements $h \in \mathfrak{grt}$ is $h(x,y) + h(y,x) = 0$.

while the b-degree corresponds to the mould depth r; thus for all $r \geq 1$, the depth r part of the mould $T_w = ma\big(\tau_w(a)\big)$ is a polynomial in $u_1, \ldots, u_r$ of degree $w+1$. Furthermore, the lowest depth part of T_w appears in depth 1 and is given by

$$T_w(u_1) = ma\big(\mathrm{ad}_a^{w+1}(b)\big) = u_1^{w+1}\,. \tag{6.49}$$

It remains only to prove that $T_w(u_1, \ldots, u_r) = 0$ for all even r. For this, we apply Theorem 6.1.6 to the case $h = g_w$ and $H = G_w = ma(g_w)$. By (ii) of that theorem, we have

$$T_w = \Delta \circ \mathrm{Ad}_{ari}(invpal)(G_w)\,. \tag{6.50}$$

Therefore for each $r \geq 1$ we have

$$\Delta^{-1}(T_w)(u_1, \ldots, u_r) = \frac{T_w(u_1, \ldots, u_r)}{u_1 \cdots u_r(u_1 + \cdots + u_r)} = \mathrm{Ad}_{ari}(invpal)(G_w)(u_1, \ldots, u_r)\,. \tag{6.51}$$

By (i) of Theorem 6.1.6, the mould $\mathrm{Ad}_{ari}(invpal)(G_w)$ is bialternal, so the rational mould in the middle term is bialternal. The total degree of this rational function is $w-r$, which is odd whenever r is even. Thus, by Theorem 6.1.6 (iv), the mould T_w is zero in all even depths r. This concludes the proof of the Proposition. □

Corollary 6.2.3 (Theorem 5.4.1 (ii))**.**

(i) The minimal degree part of the Lie series $\tau_w(a)$ is equal to $\mathrm{ad}_a^{w+1}(b)$, so the minimal degree part of τ_w is ϵ_{w+1}. The minimal degree part of σ_w is given by $-\frac{1}{(w-1)!}\epsilon_{w+1}^{(w-1)}$.

(ii) There are no terms of degree $< w+2$ and no terms of even degree in the Lie series $\tau_w(a)$, $\sigma_w(a)$ and their partners. For all odd $n \geq w+2$, the terms of $\tau_w(a)$ (resp. $\sigma_w(b)$) all have b-degree (resp. a-degree) equal to $n-w-1$ and constant a-degree (resp. constant b-degree) equal to $w+1$.

Proof. (i) We saw in (6.48) that the lowest degree of $\tau_w(a)$ is $w+2$ and $\tau_w(a)|_{w+2} = \mathrm{ad}_a^{w+1}(b)$, which is also equal to $\epsilon_w(a)$ by (5.2). The switch formula is given in (5.13).

(ii) The statement is a direct translation of the corresponding statement of the previous proposition into terms of the non-commutative variables a, b. The minimal degree of τ_w and σ_w as a derivations is $w+1$ by part (i), so the minimal degree of the Lie series $\tau_w(a)$ and $\sigma_w(a)$ is $w+2$. For the other terms, the map ma sends a polynomial $h \in \mathbb{Q}\langle c_1, c_2, \ldots\rangle$ (with $c_i = \mathrm{ad}_a^{i-1}(b)$) of homogeneous degree n in a, b and homogeneous depth r to a mould $ma(h)$ concentrated in depth r of homogeneous degree $n-r$ in the variables $u_1, \ldots, u_r$. Since the degree of $T_w(u_1, \ldots, u_r)$ is always $w+1$ by the previous Proposition, the a-degree of every term of $\tau_w(a)$ is $w+1$. The depth r part of the mould T_w corresponds to the b-degree r part of the power series $\tau_w(a)$. We first observe that if r is even then $T_w(u_1, \ldots, u_r) = 0$ by the previous proposition, so all terms of $\tau_w(a)$ of even b-degree r are zero, but these are precisely all the terms of total degree $w+1+r$, which are all of the even-degree terms. If we have a term $\tau_w(a)$ of odd total degree n, then since it has a-degree $w+1$ its b-degree is equal to $n-w-1$. This concludes the proof for $\tau_w(a)$ and the switch gives the analogous result for $\sigma_w(b)$ with b-degree $w+1$ and a-degree $n-w-1$. □

Proposition 6.2.4. *For each odd $w \geq 3$, the mould $T_w = ma\big(\tau_w(a)\big)$ is entirely determined by its parts of depth $r \leq w-1$.*

Proof. By Theorem 6.1.6 (ii), the mould $\Delta^{-1}T_w$ is equal to $\mathrm{Ad}_{ari}(invpal)(G_w)$ where $G_w = ma(g_w)$ and g_w is the canonical polynomial in genus zero. For any moulds $P \in GARI$ and $A \in ARI$, set $L = \log_{ari}(P)$ and recall the adjoint operator formula (6.14). Since L has no constant term, taking the ari-bracket with L increases the depth, so the adjoint operator formula shows that for any given depth r, only the terms of A of depth $\leq r$ contribute to the depth r part of $\mathrm{Ad}_{ari}(P)(A)$. Now let $A = \mathrm{Ad}_{ari}(invpal)(G_w)$ and $P = pal$, so that

$$\mathrm{Ad}_{ari}(P)(A) = \mathrm{Ad}_{ari}(pal)\big(\mathrm{Ad}_{ari}(invpal)(G_w)\big) = G_w\,. \tag{6.52}$$

Since g_w is a Lie polynomial of degree w it has no terms of depth $\geq w$, so the same is true for the associated mould $G_w = ma(g_w)$. Thus, G_w is determined entirely by its parts of depth $\leq w-1$, which in turn by the adjoint action formula are determined entirely by the parts of $A = \mathrm{Ad}_{ari}(invpal)(G_w)$ in depths $\leq w-1$. The parts of T_w of depth $\leq w-1$ determine those of $A = \mathrm{Ad}_{ari}(invpal)(G_w)$ by applying Δ^{-1}, and the parts of A of depths $\leq w-1$ then determine G_w up to depth $w-1$ by the adjoint action formula (6.52) – but this is all of G_w, which then in turn determines all of T_w by the formula

$$T_w = \Delta \circ \mathrm{Ad}_{ari}(invpal)(G_w)\,, \tag{6.53}$$

concluding the proof of the proposition. □

Corollary 6.2.5 (Theorem 5.4.1 (iii))**.** *Both of the derivations τ_w and σ_w are entirely determined by their parts of degree $\leq 2w-1$ (as derivations).*

Proof. By the above Proposition, T_w is entirely determined by its parts of depth $\leq w-1$, so the same holds for the Lie series $\tau_w(a)$. But we saw above that for all $r \geq 1$ the b-degree r part of the Lie series $\tau_w(a)$ is of polynomial degree $w+r+1$ in a and b, so in particular the b-degree $w-1$ part of $\tau_w(a)$ is of degree $2w$. Saying that $\tau_w(a)$ is determined by its parts of b-degree $\leq w-1$ is equivalent to saying that it is determined by its parts of total degree $\leq 2w$. Since $\tau_w([a,b]) = 0$ by Corollary 6.2.1, knowing $\tau_w(a)$ determines τ_w completely. The part of $\tau_w(a)$ of given polynomial degree n corresponds to the part of τ_w of degree $n-1$ as a derivation; thus the derivation τ_w is entirely determined by its parts of degree $\leq 2w-1$, and the same holds for σ_w. □

6.3 Proof of Theorem 5.4.1 (iv)-(vi)

In this section, we use properties of the $\mathfrak{sl}_2$ algebra in Definition 5.1.3 with generators $\epsilon_0, \epsilon_0^\vee, \mathrm{h}$ to prove parts (iv)-(vi) of Theorem 5.4.1.

Since the element $\mathrm{h} = [\epsilon_0, \epsilon_0^\vee] \in \mathfrak{sl}_2 \subset \mathrm{Der}^0\mathrm{Lie}[a,b]$ acts by $\mathrm{h}(a) = -a$ and $\mathrm{h}(b) = b$, any derivation δ of $\widehat{\mathrm{Lie}}[a,b]$ of homogeneous a-degree α and b-degree β is an eigenvector for h, with eigenvalue given by

$$[\mathrm{h}, \delta] = (\beta - \alpha)\delta\,. \tag{6.54}$$

In particular, for the action of h on $\mathfrak{u}$, we have $[\mathrm{h}, \epsilon_k^{(j)}] = (2j{+}2{-}k)\epsilon_k^{(j)}$ from (5.11), so h has eigenvalues covering the spectrum of values $-k{+}2, -k{+}4, \ldots, -2, 0, 2, \ldots, k{-}4, k{-}2$ within the $(k-1)$-dimensional irreducible representations $\{\epsilon_k^{(j)},\ j = 0, 1, \ldots, k-2\}$ of $\mathfrak{sl}_2$ at fixed k. Similarly, $(r-1)$-dimensional irreducible subrepresentations in $\mathfrak{u}$ built from brackets of $\epsilon_{k_1}^{(j_1)}\epsilon_{k_2}^{(j_2)}\ldots\epsilon_{k_m}^{(j_m)}$ will have the spectrum of h-eigenvalues $-r{+}2, -r{+}4, \ldots, -2, 0, 2, \ldots, r{-}4, r{-}2$, always including the eigenvalue zero since r is even as will become clear from the discussion around (7.3).

By $[\mathrm{h}, \epsilon_0] = 2\epsilon_0$ and $[\mathrm{h}, \epsilon_0^\vee] = -2\epsilon_0^\vee$, adjoint action of ϵ_0 and $\epsilon_0^\vee$ shifts the h eigenvalue of any derivation $\delta \in \mathrm{Der}^0\widehat{\mathrm{Lie}}[a,b]$ (not necessarily $\delta \in \mathfrak{u}$) by 2 and -2, respectively (except for highest- and lowest-weight vectors annihilated by ad_{ϵ_0} and $\mathrm{ad}_{\epsilon_0^\vee}$, respectively).

Lemma 6.3.1. *By the above spectra of* h *eigenvalues in irreducible representations of* $\mathfrak{sl}_2$ *and the action (5.12) as well as the fact that* $\mathrm{ad}_{\epsilon_0}\epsilon_k^{(j)} = \epsilon_k^{(j+1)}$ *and* $\epsilon_k^{(k-1)} = 0$, *we have:*

(i) for any $Y \in \mathrm{ad}_{\epsilon_0}\mathfrak{u}$, *the equation* $\mathrm{ad}_{\epsilon_0}X = Y$ *has a unique solution* $X \in \mathrm{ad}_{\epsilon_0^\vee}\mathfrak{u}$. *In particular,* ad_{ϵ_0} *has no kernel within eigenspaces at negative eigenvalues of* h.

(ii) for any $Y \in \mathrm{ad}_{\epsilon_0^\vee}\mathfrak{u}$, *the equation* $\mathrm{ad}_{\epsilon_0^\vee}X = Y$ *has a unique solution* $X \in \mathrm{ad}_{\epsilon_0}\mathfrak{u}$. *In particular,* $\mathrm{ad}_{\epsilon_0^\vee}$ *has no kernel at positive eigenvalues of* h.

6.3.1 Proof of Theorem 5.4.1 (iv)

For any term of σ_w of total degree n, since by Theorem 5.4.1 (ii) the b-degree is w, the a-degree must be $n - w$, and thus by (6.54) this term is an h-eigenvector with h-eigenvalue equal to $2w - n$. Thus any term of σ_w of bihomogeneous degree in a and b and total degree n is an eigenvector for h, and we have:

$$\begin{aligned} &\text{if } n < 2w, \text{ the eigenvalue of h is strictly positive,}\\ &\text{if } n = 2w, \text{ the eigenvalue of h is zero,}\\ &\text{if } n > 2w, \text{ the eigenvalue of h is negative.} \end{aligned} \tag{6.55}$$

Lemma 6.3.2 (Theorem 5.4.1 (iv))**.** *The derivation* σ_w *has no highest-weight vectors in degrees* $n > 2w$.

Proof. Since ad_{ϵ_0} has no kernel at negative h-eigenvalues by Lemma 6.3.1 (i), the infinite Lie series of geometric contributions to σ_w above key degree $2w$ does not involve any highest-weight vectors. ∎

6.3.2 Proof of Theorem 5.4.1 (v) and (vi)

We shall next prove parts (v) and (vi) of Theorem 5.4.1 based on Theorem 5.2.1. In a notation where

$$\mathfrak{g} := \mathfrak{u} \rtimes \mathfrak{sl}_2 \,, \tag{6.56}$$

and $\mathcal{S}$ denotes the free Lie algebra of zeta generators σ_w, Theorem 5.2.1 implies that

$$[\mathfrak{g}, \mathcal{S}] \subset \mathfrak{g} \,. \tag{6.57}$$

Following the notation p_d for degree-d parts of polynomials p in a, b, we shall write $(\sigma_w)_d$ for the degree-d part of genus one zeta generators, so that in particular $\sigma_w^{\rm key} = (\sigma_w)_{2w}$.

Proposition 6.3.3 (Theorem 5.4.1 (v) and (vi))**.**

(i) All terms of σ_w in degrees $\neq 2w$ lie in $\mathfrak{u}$, but $\sigma_w^{\rm key} \notin \mathfrak{u}$.

(ii) The terms of σ_w in key degree $2w$ that lie in irreducible $\mathfrak{sl}_2$ representations of dimension ≥ 3 lie in $\mathfrak{u}$.

(iii) The brackets $[z_w, \epsilon_k]$ of the $\mathfrak{sl}_2$-invariant part z_w of σ_w lie in $\mathfrak{u}$.

Proof. (i) Recall from Theorem 5.4.1 (ii) that every term of σ_w is of b-degree w and that the minimum total degree of any term is given by $n = w+1$. Let

$$\sigma_w = \sum_{n=w+1}^{\infty} (\sigma_w)_n \tag{6.58}$$

denote the expansion of σ_w according to total degree. Then by (6.54), for each $n \geq w+1$, we have

$$[\mathrm{h}, (\sigma_w)_n] = (2w-n)(\sigma_w)_n \,. \tag{6.59}$$

Note that, instead of (6.57), we actually have the stronger statement

$$[\mathfrak{g}, \mathcal{S}] \subset \mathfrak{u} \tag{6.60}$$

since the brackets on the left-hand cannot have any terms of degree zero and $\mathfrak{u}$ is the part of $\mathfrak{g}$ of degree > 0. Thus, the bracket $[\mathrm{h}, \sigma_w]$ must lie in $\mathfrak{u}$ and indeed each separate term $[\mathrm{h}, (\sigma_w)_n]$ must already lie in $\mathfrak{u}$ since there are no linear relations between terms of different degree. Hence, by (6.59), we must have

$$(2w-n)(\sigma_w)_n \in \mathfrak{u} \tag{6.61}$$

for all $n \geq w+1$, i.e. for all terms of σ_w. In particular, whenever $2w - n \neq 0$, (6.61) implies that $(\sigma_w)_n \in \mathfrak{u}$. Terms of σ_w not in $\mathfrak{u}$ can thus only occur when $n = 2w$, i.e. in key degree.

The fact that $\sigma_w^{\text{key}} \notin \mathfrak{u}$ follows directly from Theorem 5.2.1, since if σ_w^{key} lied in $\mathfrak{u}$ then we would have $\sigma_w \in \mathfrak{u}$, so $\mathfrak{u}$ together with the σ_w could not generate a semi-direct product as in Theorem 5.2.1 (ii).

(ii) Once again, by (6.60), any bracket of $\mathfrak{sl}_2$ elements and σ_w, and therefore in particular $[\epsilon_0, (\sigma_w)_{2w}]$ must lie in $\mathfrak{u}$. If we decompose

$$(\sigma_w)_{2w} = \sum_{\text{odd } d\geq 1} (\sigma_w)_{2w}^{(d)}\,, \tag{6.62}$$

where $(\sigma_w)_{2w}^{(d)}$ collects the key-degree terms in σ_w that lie in d-dimensional irreducible representations of $\mathfrak{sl}_2$, we must then have

$$[\epsilon_0, (\sigma_w)_{2w}^{(d)}] \in \mathfrak{u} \tag{6.63}$$

separately for each (odd) $d \geq 1$. When $d \geq 3$, the terms $[\epsilon_0, (\sigma_w)_{2w}^{(d)}] \in \mathfrak{u}$ are non-zero since highest-weight vectors of ($d \geq 3$)-dimensional $\mathfrak{sl}_2$ representations have h-eigenvalue ≥ 2. Then, thanks to the equality[12]

$$(\sigma_w)_{2w}^{(d)} = \frac{4}{(d-1)(d+1)}[\epsilon_0^\vee, [\epsilon_0, (\sigma_w)_{2w}^{(d)}]]\,, \tag{6.64}$$

we see that for $d \geq 3$, the term $(\sigma_w)_{2w}^{(d)}$ itself lies in $\mathfrak{u}$ since $\mathfrak{u}$ is an $\mathfrak{sl}_2$-module by Theorem 5.2.1.

When $d = 1$, the term $[\epsilon_0, (\sigma_w)_{2w}^{(1)}] = 0$ and therefore we cannot use (6.63) to conclude that $(\sigma_w)_{2w}^{(1)}$ lies in $\mathfrak{u}$; indeed we know that it cannot lie in $\mathfrak{u}$ since otherwise all of σ_w would, contradicting (i). This proves that the arithmetic terms z_w of σ_w form a one-dimensional $\mathfrak{sl}_2$ representation in key degree.

Finally, (iii) follows directly from (6.60), since this shows that $[\epsilon_k, \sigma_w] \in \mathfrak{u}$ and z_w is the only term of σ_w not already in $\mathfrak{u}$. $\square$

7 Recursive high-order computations of σ_w and $[z_w, \epsilon_k]$

In this section, we combine representation theory of $\mathfrak{sl}_2$ with Theorem 5.4.1, particularly part (vii) recalled below, to perform explicit high-order computations of σ_w and $[z_w, \epsilon_k]$ in terms of nested brackets of $\epsilon_k^{(j)}$.

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[12]The prefactor follows from the fact that the $\mathfrak{sl}_2$ properties of $[\epsilon_0, (\sigma_w)_{2w}^{(d)}]$ are identical to $\epsilon_{d+1}^{(\frac{d+1}{2})}$, where the action of the lowering operator $\text{ad}_{\epsilon_0^\vee}$ yields $\frac{1}{4}(d-1)(d+1)\epsilon_{d+1}^{(\frac{d-1}{2})}$ by (5.12).

7.1 Proof and first consequences of Theorem 5.4.1 (vii)

Proposition 7.1.1 (Theorem 5.4.1 (vii))**.** *Let* $\mathrm{BF}_k := \frac{\mathrm{B}_k}{k!}$ *for* $k \geq 2$*, and set*

$$N := -\epsilon_0 + \sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k\epsilon_k\,. \tag{7.1}$$

Then for all odd $w \geq 3$ *we have*

$$[N, \sigma_w] = 0 \in \mathrm{Der}^0\widehat{\mathrm{Lie}}[a, b]\,. \tag{7.2}$$

Proof. The proof of this result is given in section 27 of [21] based on sections 12 and 13 of [79], so we simply indicate the essential argument here. In the framework set forth in Remark 5.2.2, we noted that the two profinite groups $\widehat{\mathrm{SL}}_2(\mathbb{Z})$ and the absolute Galois group $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ both act naturally as automorphisms on the profinite fundamental group $\hat{\pi}_1(E_\infty)$ of the nodal elliptic curve, where $\mathrm{SL}_2(\mathbb{Z})$ is identified with the fundamental group of the moduli space $\mathcal{M}_{1,1}$. There is a distinguished element in $\widehat{\mathrm{SL}}_2(\mathbb{Z})$ on which $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ acts via its abelian quotient $\mathrm{Gal}(\overline{\mathbb{Q}}^{\mathrm{ab}}/\mathbb{Q})$: this is the element corresponding to a small loop around the degenerate point $\tau = i\infty$ in the moduli space (or as Hain–Matsumoto describe it, a small loop around $q = 0$ in the q-disk where $q = e^{2\pi i\tau}$). Thus in the pro-unipotent version, or rather the associated Lie algebra version, the arithmetic part $\mathcal{S}$ corresponding to the Galois action commutes with the image of this element in the Lie algebra $\mathfrak{u} \rtimes \mathfrak{sl}_2$. There are various ways of showing that this image is equal to the element N defined in (7.1); the method used in section 12 of [79] is to identify it as the residue at $q = 0$ of the restriction of the KZB connection (see appendix A) to a first order neighborhood of the degenerate nodal curve. ☐

In the remainder of this section, the commutation relation (7.2) will be applied to recursively determine the *infinite* series expansions of σ_w as in (5.46) to (5.50) from the *finitely* many terms in degree $\leq 2w$. The finitely many contributions to σ_w not yet determined by (7.2) are precisely the highest-weight vectors of $\mathfrak{sl}_2$, i.e. the elements in the kernel of ad_{ϵ_0}. By Theorem 5.4.1 (iv), these highest-weight-vector contributions to σ_w occur only up to and including key degree $2w$ which explains the finite number of them for each w.

For example, when $w = 3$, the key degree is 6 and feeding the highest-weight vector contributions $-\frac{1}{2}\epsilon_4^{(2)}$ and z_3 into (7.2) determines all of σ_3, see (7.22) below for the exact result. When $w = 5$, the highest-weight vectors $-\frac{1}{24}\epsilon_6^{(4)}$, $-\frac{5}{48}[\epsilon_4^{(1)}, \epsilon_4^{(2)}]$ and z_5 occurring in the low-degree part of σ_5 feed into (7.2) and determine all of σ_5.[13]

Our construction of σ_w from finitely many highest-weight vectors will be recursive in the *modular depth* of its geometric contributions which we define as follows:

[13] The analogous highest-weight vectors in the expansion (5.49) that completely determine σ_7 are given by $-\frac{1}{720}\epsilon_8^{(6)}$ at degree 8, by $\frac{7}{1152}([\epsilon_4^{(2)}, \epsilon_6^{(3)}] - [\epsilon_4^{(1)}, \epsilon_6^{(4)}])$ at degree 10, by $\frac{1}{13824}([\epsilon_6^{(1)}, \epsilon_6^{(4)}] - [\epsilon_6^{(2)}, \epsilon_6^{(3)}])$ and $-\frac{661}{57600}([\epsilon_4^{(1)}, [\epsilon_4^{(1)}, \epsilon_4^{(2)}]] + [\epsilon_4^{(2)}, [\epsilon_4^{(2)}, \epsilon_4]])$ at degree 12 and finally z_7 at key degree 14.

Definition 7.1.2. Nested brackets $[[\ldots[[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}], \epsilon_{k_3}^{(j_3)}], \ldots], \epsilon_{k_r}^{(j_r)}]$ of r derivations $\epsilon_k^{(j)}$ in $\mathfrak{u}$ are said to have *modular depth* r. The modular depth forms a natural increasing filtration on $\mathfrak{u}$, but not a grading, as shown for example by the Pollack relation (5.19) which can be viewed as an equality between linear combinations of terms of modular depth 2 with two terms of modular depth 3.

In addition to the infinitely many terms in the series expansion of σ_w above key degree, the recursive method of section 7.3 will completely determine the explicit form of the brackets $[z_w, \epsilon_k]$ of the arithmetic contributions z_w to the zeta generators. We reiterate that, by Theorem 5.4.1 (v) and (vi), the non-geometric part z_w of σ_w is concentrated in a one-dimensional $\mathfrak{sl}_2$ representation at key degree $2w$ and gives rise to brackets $[z_w, \epsilon_k] \in \mathfrak{u}$.

7.2 $\mathfrak{sl}_2$ prerequisites

We start by organizing $\mathfrak{u}$ into representations of the subalgebra $\mathfrak{sl}_2$ of $\mathrm{Der}^0\mathrm{Lie}[a, b]$, and describing its irreducible pieces; in particular we determine the highest- and lowest-weight vectors of each one.

In view of the nilpotency $\mathrm{ad}_{\epsilon_0}^{k-1}\epsilon_k = 0$ (see (5.8)), the non-zero $\epsilon_k^{(j)} = \mathrm{ad}_{\epsilon_0}^{j}\epsilon_k$ for fixed even k and $j = 0, 1, \ldots, k-2$ form a $(k-1)$-dimensional irreducible representation of $\mathfrak{sl}_2$, which we denote by $V(\epsilon_k)$. The generators $\epsilon_0, \epsilon_0^\vee, \mathrm{h}$ of $\mathfrak{sl}_2$ permute the elements of $V(\epsilon_k)$ simply by $\mathrm{ad}_{\epsilon_0}\epsilon_k^{(j)} = \epsilon_k^{(j+1)}$, (5.11) and (5.12), identifying ad_{ϵ_0} and $\mathrm{ad}_{\epsilon_0^\vee}$ as the raising and lowering operators for the eigenvalues of h, respectively. All irreducible representations of $\mathfrak{sl}_2$ inside $\mathfrak{u}$ are formed from nested commutators of the $\epsilon_k^{(j)}$, and they are all isomorphic (as $\mathfrak{sl}_2$-representations) to some $V(\epsilon_k)$ for even $k \geq 2$. Note that each odd-dimensional $\mathfrak{sl}_2$-representation occurs infinitely many times in $\mathfrak{u}$, and they can be arranged by modular depth.

The collections of commutators $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$ for fixed k_1, k_2 and $j_i = 0, 1, \ldots, k_i - 2$ sit inside the reducible tensor-product representations $V(\epsilon_{k_1}) \otimes V(\epsilon_{k_2})$ of $\mathfrak{sl}_2$ which can be decomposed into the following $(r-1)$-dimensional irreducible representations $V(\epsilon_r)$ of $\mathfrak{sl}_2$:

$$V(\epsilon_{k_1}) \otimes V(\epsilon_{k_2}) = \bigoplus_{\substack{r=|k_1-k_2|+2 \\ r \in 2\mathbb{Z}}}^{k_1+k_2-2} V(\epsilon_r)\,. \tag{7.3}$$

Since r is restricted to even values, the dimensions of the irreducible representations of $\mathfrak{sl}_2$ in iterated tensor products of $V(\epsilon_{k_i})$ are always odd.

7.2.1 Projectors to lowest-weight vectors

The projection of the commutators $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$ at modular depth two into the irreducible representations $V(\epsilon_r)$ on the right-hand side of (7.3) is implemented by

$$t^d(\epsilon_{k_1}, \epsilon_{k_2}) := \frac{(d-2)!}{(k_1-2)!(k_2-2)!} \sum_{i=0}^{d-2} (-1)^i \frac{(k_1-2-i)!(k_2-d+i)!}{i!(d-2-i)!} [\epsilon_{k_1}^{(i)}, \epsilon_{k_2}^{(d-2-i)}] \tag{7.4}$$

with $d = \frac{1}{2}(k_1 + k_2 - r + 2)$ and therefore $2 \leq d \leq \min(k_1, k_2)$. In case of $k_1 = k_2$, the $t^d(\epsilon_k, \epsilon_k)$ at even values of d vanish.

The outcomes $t^d(\epsilon_{k_1}, \epsilon_{k_2})$ of the projectors in (7.4) are lowest-weight vectors (see Definition 5.1.3) of the $V(\epsilon_r)$ in the tensor product (7.3). The rest of the $(r-1)$-dimensional irreducible representations in $\mathfrak{u}$ at modular depth two is obtained from $\mathrm{ad}_{\epsilon_0}^j t^d(\epsilon_{k_1}, \epsilon_{k_2})$ with $j = 0, 1, \ldots, r-2$ and terminates due to $\mathrm{ad}_{\epsilon_0}^{r-1} t^d(\epsilon_{k_1}, \epsilon_{k_2}) = 0$.

Since $t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2})$ is a lowest-weight vector it can be inserted on the same footing as ϵ_r with $r = k_1 + k_2 - 2d_1 + 2$ into another operation (7.4). For instance,

$$t^{d_2}(\epsilon_{k_3}, t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2})) = \frac{(d_2-2)!}{(k_3-2)!(r-2)!} \sum_{i=0}^{d_2-2} (-1)^i \frac{(k_3-2-i)!(r-d_2+i)!}{i!(d_2-2-i)!} \times [\epsilon_{k_3}^{(i)}, \mathrm{ad}_{\epsilon_0}^{d_2-2-i} t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2})] \tag{7.5}$$

is the lowest-weight vector of a $(k_1 + k_2 + k_3 - 2d_1 - 2d_2 + 3)$-dimensional irreducible $\mathfrak{sl}_2$ representation in the triple tensor product $V(\epsilon_{k_1}) \otimes V(\epsilon_{k_2}) \otimes V(\epsilon_{k_3})$ which may be decomposed into irreducibles by iterating (7.3). Iterations of the t^d projectors (7.4) as exemplified in (7.5) are instrumental for compactly representing the contributions to $[z_w, \epsilon_k]$ at modular depth three in section 7.4.2 below.

7.2.2 Projectors to highest-weight vectors

One can similarly generate highest-weight vectors of the the irreducible representations $V(\epsilon_r)$ in $V(\epsilon_{k_1}) \otimes V(\epsilon_{k_2})$ and tensor products at higher modular depth via

$$s^d(\epsilon_{k_1}, \epsilon_{k_2}) := \frac{(d-2)!}{(k_1-2)!(k_2-2)!} \sum_{i=0}^{d-2} (-1)^i [\epsilon_{k_1}^{(k_1-2-i)}, \epsilon_{k_2}^{(k_2-d+i)}] \tag{7.6}$$

where again $d = \frac{1}{2}(k_1 + k_2 - r + 2)$, as long as $2 \leq d \leq \min(k_1, k_2)$. Nevertheless, we will see that an extension of (7.6) to $d > \min(k_1, k_2)$ will be useful to bring certain contributions to σ_w into a convenient form, though the highest-weight vector property $[\epsilon_0, s^d(\epsilon_{k_1}, \epsilon_{k_2})] = 0$ only holds for $d \leq \min(k_1, k_2)$. Since the entries $\epsilon_{k_1}, \epsilon_{k_2}$ of the s^d-operation in (7.6) are lowest-weight vectors, the nested brackets relevant to modular depth $m \geq 3$ are generated by m iterations of t^{d_i} and a single s^d operation for the outermost bracket. For instance,

$$s^{d_2}(\epsilon_{k_3}, t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2})) = \frac{(d_2-2)!}{(k_3-2)!(r-2)!} \sum_{i=0}^{d_2-2} (-1)^i [\epsilon_{k_3}^{(k_3-2-i)}, \mathrm{ad}_{\epsilon_0}^{k_2-d_2+i} t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2})] \tag{7.7}$$

at suitable values for d_1, d_2 (with $r = k_1 + k_2 - 2d_1 + 2$) generate all highest-weight vectors of the irreducible $\mathfrak{sl}_2$ representations in $V(\epsilon_{k_1}) \otimes V(\epsilon_{k_2}) \otimes V(\epsilon_{k_3})$. In general, iterations of $s^{d_{m-1}} t^{d_{m-2}} \ldots t^{d_1}$ conveniently capture the highest-weight-vector contributions to σ_w at each modular depth that are not yet determined by the recursion below based on $[N, \sigma_w] = 0$ (see Theorem 5.4.1 (vii)).

7.2.3 $\mathfrak{sl}_2$ representations of Pollack relations

The Pollack relations among $\epsilon_k^{(j)}$ with $k \geq 4$ and $0 \leq j \leq k-2$ in Remark 5.1.6 fall into irreducible $\mathfrak{sl}_2$ representations of dimension ≥ 11.[14] As exemplified by the second relation in (5.18), Pollack relations generically mix contributions of different modular depths ≥ 2.

7.3 Recursive higher-order computations of σ_w and $[z_w, \epsilon_k]$

Based on the vanishing of $[N, \sigma_w]$ in section 7.1 and the $\mathfrak{sl}_2$ prerequisites of section 7.2, we shall now set up the recursive high-order computations of σ_w and $[z_w, \epsilon_k]$ in terms of nested brackets of $\epsilon_k^{(j)}$. For this purpose, we parametrize the desired expressions according to modular depth.

Definition 7.3.1. Given that $\sigma_w - z_w$ and $[z_w, \epsilon_k]$ both lie in $\mathfrak{u}$ for any odd $w \geq 3$ and even $k \geq 4$ by Theorem 5.4.1 (v) and (vi), we expand

$$\begin{aligned} \sigma_w &= z_w + \sigma_w^{\{1\}} + \sigma_w^{\{2\}} + \sigma_w^{\{3\}} + \ldots + \sigma_w^{\{w\}} , \\ [z_w, \epsilon_k] &= [z_w, \epsilon_k]^{\{1\}} + [z_w, \epsilon_k]^{\{2\}} + [z_w, \epsilon_k]^{\{3\}} + \ldots + [z_w, \epsilon_k]^{\{w+1\}} , \end{aligned} \tag{7.8}$$

where $\sigma_w^{\{m\}}$ and $[z_w, \epsilon_k]^{\{m\}}$ refer to combinations of $[[\ldots[[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}], \epsilon_{k_3}^{(j_3)}], \ldots], \epsilon_{k_m}^{(j_m)}] \in \mathfrak{u}$ at modular depth $m = 1, 2, \ldots, w+1$. The properties of the arithmetic derivations $z_w \in \mathrm{Der}^0 \widehat{\mathrm{Lie}}[a, b]$ outside $\mathfrak{u}$ can be found in Theorem 5.4.1 (vi) — a- and b-degree w and vanishing commutators $[z_w, \epsilon_0] = [z_w, \epsilon_0^\vee] = 0$.

Remark 7.3.2. The maximum modular depth w of σ_w and $w+1$ of $[z_w, \epsilon_k]$ in (7.8) both follow from the fact that each ϵ_m with $m \geq 0$ has b-degree 1: the b-degrees w of σ_w (see Theorem 5.4.1 (ii)) and $w+1$ of $[z_w, \epsilon_k]$ are incompatible with modular depths $\sigma_w^{\{m \geq w+1\}}$ and $[z_w, \epsilon_k]^{\{m \geq w+2\}}$. The well-known vanishing of $[z_w, \epsilon_k]^{\{1\}}$ [26, 27, 21] follows from the fact that only expression in $\mathfrak{u}$ compatible with its a- and b-degrees is $\epsilon_{2w+k}^{(w)}$ which violates the lowest-weight-vector property of z_w and ϵ_k.

Remark 7.3.3. We recall that generic Pollack relations among $\epsilon_k^{(j)}$ with $k \geq 4$ and $0 \leq j \leq k-2$ in Remark 5.1.6 relate nested brackets of different modular depth ≥ 2. Accordingly, the individual contributions $\sigma_w^{\{m \geq 2\}}$ and $[z_w, \epsilon_k]^{\{m \geq 2\}}$ to the right-hand side of (7.8) are usually not well-defined before specifying a scheme of applying those Pollack relations that mix modular depths.[15] We will specify a choice of $\sigma_w^{\{2\}}$ and $[z_w, \epsilon_k]^{\{2\}}$ for all odd $w \geq 3$ in (7.15)

[14] More specifically, Pollack relations whose relative factors in the modular-depth-two contributions $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$ are governed by holomorphic cusp forms of modular weight w [26] fall into irreducible $\mathfrak{sl}_2$ representations of dimension $w-1$.

[15] For instance, the image of the second relation in (5.18) under $\mathrm{ad}_{\epsilon_0}^{10}$ can be used to convert contributions $\sim s^3(\epsilon_4, \epsilon_{12}), s^3(\epsilon_6, \epsilon_{10})$ and $s^3(\epsilon_8, \epsilon_8)$ to $\sigma_{13}^{\{2\}}$ into contributions $\sim [\epsilon_4^{(2)}, [\epsilon_4^{(2)}, \epsilon_8^{(6)}]]$ and $[\epsilon_6^{(4)}, [\epsilon_6^{(4)}, \epsilon_4^{(2)}]]$ to $\sigma_{13}^{\{3\}}$. Similarly, the coefficient of $t^4(\epsilon_4, \epsilon_{14})$ in $[z_3, \epsilon_{12}]^{\{2\}}$ can be modified through Pollack relations of degree 18 at the cost of extra terms in all of $[z_3, \epsilon_{12}]^{\{2\}}$, $[z_3, \epsilon_{12}]^{\{3\}}$ and $[z_3, \epsilon_{12}]^{\{4\}}$.

and (7.18) below which eliminates some of the ambiguities in $\sigma_w^{\{3\}}$ and $[z_w, \epsilon_k]^{\{3\}}$ (those that descend from Pollack relations involving terms of modular depth two). Nevertheless, the recursive relations among $\sigma_w^{\{m\}}$ to be derived below are valid for any scheme of applying Pollack relations that mix different modular depths as long as the same choice is consistently applied to all modular depths $m \geq 2$.

In the companion paper [8], we study uplifts of zeta generators $\sigma_w \to \hat{\sigma}_w$ which no longer act on $\widehat{\mathrm{Lie}}[a,b]$ and where the $\epsilon_k^{(j)}$ in their series expansion in $\mathfrak{u}$ are promoted to free-algebra generators $\mathrm{e}_k^{(j)}$ with $k \geq 4$ and $0 \leq j \leq k-2$. The expansion of the uplifted $\hat{\sigma}_w$ in terms of $\mathrm{e}_k^{(j)}$ is determined from considerations of non-holomorphic modular forms and does not share the ambiguities from Pollack relations. Accordingly, the uplifted $\hat{\sigma}_w$ induce preferred representations of the $\sigma_w^{\{m\}}$ and $[z_w, \epsilon_k]^{\{m\}}$ at $m = 2$ and partially at $m = 3$ which will be followed in section 7.4.

With the notation of Definition 7.3.1 for the contributions of fixed modular depth m, we organize the property $[N, \sigma_w] = 0$ as written in (7.2) according to modular depth

$$\begin{aligned} 0 = [N, \sigma_w] = &-[\epsilon_0, \sigma_w^{\{1\}} + \sigma_w^{\{2\}} + \ldots + \sigma_w^{\{w\}}] \\ &+ \sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k \Big([\epsilon_k, \sigma_w^{\{1\}}] + [\epsilon_k, \sigma_w^{\{2\}}] + \ldots + [\epsilon_k, \sigma_w^{\{w\}}] \\ &\qquad - [z_w, \epsilon_k]^{\{1\}} - [z_w, \epsilon_k]^{\{2\}} - \ldots - [z_w, \epsilon_k]^{\{w+1\}} \Big) , \end{aligned} \tag{7.9}$$

where $\mathrm{BF}_k \coloneqq \frac{\mathrm{B}_k}{k!}$, and we have used $\mathfrak{sl}_2$ invariance $[\epsilon_0, z_w] = 0$.

Proposition 7.3.4. *Upon isolating the contributions to (7.9) at fixed modular depth $m = 1, 2, \ldots, w+1$, we deduce*

$$[\epsilon_0, \sigma_w^{\{m\}}] + \sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k [z_w, \epsilon_k]^{\{m\}} = \sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k [\epsilon_k, \sigma_w^{\{m-1\}}] \,. \tag{7.10}$$

In particular:

(i) By $\sigma_w^{\{0\}} = 0$ and $[z_w, \epsilon_k]^{\{1\}} = 0$ (see Remark 7.3.2), the $m = 1$ instance of (7.10) enforces $[\epsilon_0, \sigma_w^{\{1\}}] = 0$. Hence, the only term in $\sigma_w^{\{1\}}$ of modular depth one compatible with the b-degree w of σ_w and (7.10) is the highest-weight vector $\sigma_w^{\{1\}} = -\frac{1}{(w-1)!}\epsilon_{w+1}^{(w-1)}$ identified in Corollary 6.2.3 (i).

(ii) Applying $\mathrm{ad}_{\epsilon_0^\vee}$ to both sides of (7.10) implies ($m = 2, 3, \ldots, w+1$)

$$[\epsilon_0^\vee, [\epsilon_0, \sigma_w^{\{m\}}]] = \sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k [\epsilon_k, [\epsilon_0^\vee, \sigma_w^{\{m-1\}}]] \tag{7.11}$$

since both z_w and ϵ_k are annihilated by $\mathrm{ad}_{\epsilon_0^\vee}$. This is the recursive approach announced earlier on to determine $\sigma_w^{\{m\}}$ from its precursor at lower modular depth $\sigma_w^{\{m-1\}}$ up *to the kernel of* $\mathrm{ad}_{\epsilon_0^\vee}\mathrm{ad}_{\epsilon_0}$*. Since* $\mathrm{ad}_{\epsilon_0^\vee}$ *is invertible on the image of* ad_{ϵ_0}*, see (ii) of Corollary 6.3.1 with* $Y \in \mathrm{ad}_{\epsilon_0^\vee}\mathfrak{u}$ *on the right-hand side composed of* $[\epsilon_k, [\epsilon_0^\vee, \sigma_w^{\{m-1\}}]] = [\epsilon_0^\vee, [\epsilon_k, \sigma_w^{\{m-1\}}]]$*, the only part of* $\sigma_w^{\{m\}}$ *which is not yet determined by (7.11) is in the kernel of* ad_{ϵ_0}*, i.e. a combination of highest-weight vectors of* $\mathfrak{sl}_2$*. By Theorem 5.4.1 (iv) proven in section 6.3.1, the highest-weight vectors in* σ_w *all occur below or at key degree. In fact,* z_w *gathers all highest-weight vectors in* σ_w^{key} *by definition, so* $\sigma_w^{\{m\}}$ *at degree* $2w$ *is free of highest-weight vectors. Hence, the missing information on* $\sigma_w^{\{m\}}$ *inaccessible from (7.11) amounts to a finite number of terms at degree* $\leq 2w-2$*.*

(iii) By inserting the expression for $\sigma_w^{\{m\}}$ *modulo highest-weight vectors found in (ii) into (7.10) and isolating terms of degree* $2w+k$*, one can solve for* $[z_w, \epsilon_k]^{\{m\}}$*. Note that contributions to* $[z_w, \epsilon_k]$ *of modular depth* m *determined from* $[N, \sigma_w] = 0$ *only depend on the highest-weight vectors in* σ_w *up to and including modular depth* $m-1$*.*

(iv) Given that $\sigma_w^{\{1\}} = -\frac{1}{(w-1)!}\epsilon_{w+1}^{(w-1)}$*, the* $m=2$ *instances of (7.10) and (7.11) can be written more explicitly as*

$$[\epsilon_0, \sigma_w^{\{2\}}] + \sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k[z_w, \epsilon_k]^{\{2\}} = -\frac{1}{(w-1)!}\sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k[\epsilon_k, \epsilon_{w+1}^{(w-1)}] \tag{7.12}$$

and

$$[\epsilon_0^\vee, [\epsilon_0, \sigma_w^{\{2\}}]] = -\frac{1}{(w-2)!}\sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k[\epsilon_k, \epsilon_{w+1}^{(w-2)}]\,. \tag{7.13}$$

Inverting the operation $\mathrm{ad}_{\epsilon_0^\vee}\mathrm{ad}_{\epsilon_0}$ *determines*

$$\begin{aligned}\sigma_w^{\{2\}} = &-\sum_{d=5}^{w}\mathrm{BF}_{d-1}s^d(\epsilon_{d-1}, \epsilon_{w+1}) - \frac{1}{2}\mathrm{BF}_{w+1}s^{w+2}(\epsilon_{w+1}, \epsilon_{w+1}) \\ &+ \sum_{k=w+3}^{\infty}\mathrm{BF}_k\sum_{j=0}^{w-2}\frac{(-1)^j\binom{k-2}{j}^{-1}}{j!(w-2-j)!}[\epsilon_{w+1}^{(w-2-j)}, \epsilon_k^{(j)}] \bmod \mathrm{Ker}(\mathrm{ad}_{\epsilon_0})\,,\end{aligned} \tag{7.14}$$

where $\bmod \mathrm{Ker}(\mathrm{ad}_{\epsilon_0})$ *refers to highest-weight vectors to be proposed in (7.18) below. All instances of the brackets* $s^d(\epsilon_{k_1}, \epsilon_{k_2})$ *defined by (7.6) that occur in (7.14) have* $d > \min(k_1, k_2)$ *and are therefore not highest-weight vectors. Upon insertion of (7.14) into (7.12) and isolating terms of degree* $2w+k$*, we reproduce the closed-form expression at modular depth two known form [21]*

$$[z_w, \epsilon_k]^{\{2\}} = \frac{\mathrm{BF}_{w+k-1}}{\mathrm{BF}_k}t^{w+1}(\epsilon_{w+1}, \epsilon_{w+k-1})\,. \tag{7.15}$$

(v) The instance of (7.10) at the maximum value $m = w+1$ *simplifies to*

$$\sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k[z_w, \epsilon_k]^{\{w+1\}} = \sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k[\epsilon_k, \sigma_w^{\{w\}}] \tag{7.16}$$

by $\sigma_w^{\{w+1\}} = 0$. Hence, the contribution to $[z_w, \epsilon_k]$ of highest modular depth $w+1$ can simply be determined from the highest-modular depth terms in σ_w by isolating the parts of degree $2w+k$ in (7.16). Validity of (7.10) at $m = 1, 2, \ldots, w+1$ — finitely many steps in the recursion in the modular depth — is sufficient for $[N, \sigma_w] = 0$, see (7.9).

Note that parts (ii) and (iii) of Proposition 7.3.4 can also be unified by the decomposition of $[\epsilon_k, \sigma_w^{\{m-1\}}]$ on the right-hand side of (7.10) into the image of ad_{ϵ_0} and the kernel of $\mathrm{ad}_{\epsilon_0^\vee}$,

$$
\begin{aligned}
[\epsilon_0, \sigma_w^{\{m\}}] &= \sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k [\epsilon_k, \sigma_w^{\{m-1\}}] \big|_{\mathrm{Im}(\mathrm{ad}_{\epsilon_0})} , \\
\sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k [z_w, \epsilon_k]^{\{m\}} &= \sum_{k=4}^{\infty} (k-1)\mathrm{BF}_k [\epsilon_k, \sigma_w^{\{m-1\}}] \big|_{\mathrm{Ker}(\mathrm{ad}_{\epsilon_0^\vee})} .
\end{aligned}
\tag{7.17}
$$

This decomposition is unique since $\mathrm{Ker}(\mathrm{ad}_{\epsilon_0^\vee})$ projects the individual terms of $[\epsilon_k, \sigma_w^{\{m-1\}}]$ to lowest-weight vectors which do not occur in the image of ad_{ϵ_0}.

7.4 Applying the recursion for $\sigma_w^{\{m\}}$ and $[z_w, \epsilon_k]^{\{m\}}$

In this section, we gather explicit results for zeta generators and commutators $[z_w, \epsilon_k]$ at modular depth $2 \leq m \leq 4$ that go considerably beyond the state of the art and found fruitful applications in the construction of non-holomorphic modular forms [8].

7.4.1 Zeta generators at modular depth two

The relation (7.13) for the modular-depth-two contributions $\sigma_w^{\{2\}}$ to the zeta generators determines the infinite series of terms in (7.14) that are not highest-weight vectors. We shall now augment these terms by a conjectural closed formula for the highest-weight vectors in $\sigma_w^{\{2\}}$ given by the first line of

$$
\begin{aligned}
\sigma_w^{\{2\}} = &-\frac{1}{2} \sum_{d=3}^{w-2} \frac{\mathrm{BF}_{d-1}}{\mathrm{BF}_{w-d+2}} \sum_{k=d+1}^{w-1} \mathrm{BF}_{k-d+1} \mathrm{BF}_{w-k+1} s^d(\epsilon_k, \epsilon_{w-k+d}) \\
&- \sum_{d=5}^{w} \mathrm{BF}_{d-1} s^d(\epsilon_{d-1}, \epsilon_{w+1}) - \frac{1}{2} \mathrm{BF}_{w+1} s^{w+2}(\epsilon_{w+1}, \epsilon_{w+1}) \\
&+ \sum_{k=w+3}^{\infty} \mathrm{BF}_k \sum_{j=0}^{w-2} \frac{(-1)^j \binom{k-2}{j}^{-1}}{j!(w-2-j)!} [\epsilon_{w+1}^{(w-2-j)}, \epsilon_k^{(j)}] .
\end{aligned}
\tag{7.18}
$$

This conjecture for the complete parts $\sigma_w^{\{2\}}$ of modular depth two is readily checked to reproduce the terms $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$ in the examples (5.46) to (5.50) at $w \leq 9$. The first line of (7.18) gathers highest-weight vectors such as $-\frac{5}{48}[\epsilon_4^{(1)}, \epsilon_4^{(2)}]$ in $\sigma_5^{\{2\}}$ and $\frac{7}{1152}([\epsilon_4^{(2)}, \epsilon_6^{(3)}] -$

$[\epsilon_4^{(1)}, \epsilon_6^{(4)}]) + \frac{1}{13824}([\epsilon_6^{(1)}, \epsilon_6^{(4)}] - [\epsilon_6^{(2)}, \epsilon_6^{(3)}])$ in $\sigma_7^{\{2\}}$[16] which have been tested for all cases of degree ≤ 22 and are in general conjectural. Note that the highest-weight-vector contributions to $\sigma_w^{\{2\}}$ in the first line of (7.18) are in one-to-one correspondence with the $\tau \to i\infty$ asymptotics of the generalized Eisenstein series $\mathrm{F}_{m,k}^{+(s)}$ in [84, 85] at $m + k + s = w + 1$ upon assembling their iterated-integral representations from the generating series of [8].

The images of the terms $s^d(\epsilon_{k_1}, \epsilon_{k_2})$ under the switch operation in Definition 5.1.4 have b-degree or depth d, and their $d = 3$ instances line up with Brown's general formula for the depth-three contributions to τ_w [27]. However, the choice of $\tau_{w\geq 11}$ in the reference does not match the *canonical* zeta generators in this work since redefinitions via nested brackets of τ_v at $v < w$ have been used in [27] to remove contributions of modular depth and b-degree three. The second and third line of (7.18) are rigorously derived by solving (7.13) and, together with the conjectural highest-weight vectors at depth $d \geq 5$ in the first line, furnish a partial generalization of Brown's result beyond depth three: On the one hand, (7.18) is claimed to capture all contributions $[\epsilon_{k_1}^{(j_1)}, \epsilon_{k_2}^{(j_2)}]$ to σ_w, regardless of their values of j_1, j_2, k_1, k_2 or depth in the sense of [27]. On the other hand, terms in σ_w at depth or b-degree d involve contributions of modular depth up to and including d, and closed formulae for $\sigma_w^{\{m\geq 3\}}$ akin to (7.18) are currently out of reach.

Note that, following the comments below (7.6), the $s^d(\epsilon_{k_1}, \epsilon_{k_2})$ in the second line of (7.18) have $d > \min(k_1, k_2)$ and are therefore not highest-weight vectors. Moreover, the expression (7.18) for contributions to σ_w of modular depth two can be rewritten in a variety of ways via Pollack relations among $\epsilon_k^{(j)}$, see Remark 7.3.3. Hence, the closed formula (7.18) for $\sigma_w^{\{2\}}$ realizes a specific choice of distributing terms between different modular depths.

7.4.2 Commutators of arithmetic derivations at modular depth three

By Proposition 7.3.4 (iii), the highest-weight vectors in σ_w at modular depth m determine the contributions to the brackets $[z_w, \epsilon_k]$ at modular depth $m+1$ via (7.10). The conjectural expressions (7.18) for $\sigma_w^{\{2\}}$ therefore translate into expressions for $[z_w, \epsilon_k]^{\{3\}}$ that generalize the simple closed formula (7.15) for terms of modular depth two.

Contributions to $[z_3, \epsilon_k]$ and $[z_5, \epsilon_k]$ at modular depth ≥ 3 and low values of k have been firstly reported in [26] and the ancillary files of [7], respectively. Moreover, the combinatorial tools developed in [26] can be used to determine more general expressions for $[z_w, \epsilon_k]$. Our conjecture (7.18) for $\sigma_w^{\{2\}}$ gives access to arbitrary $[z_w, \epsilon_k]^{\{3\}}$, but the expressions resulting from the representation-theoretic manipulations become increasingly unwieldy with growing w. Hence, we content ourselves to giving the following two infinite families of commutation relations beyond the state of the art with arbitrary even $k \geq 4$ (see (7.5) for the

[16]The analogous highest-weight vectors in $\sigma_9^{\{2\}}$ resulting from the first line of (7.18) are given by $\frac{1}{5184}([\epsilon_4^{(2)}, \epsilon_8^{(5)}] - [\epsilon_4^{(1)}, \epsilon_8^{(6)}])$ and $-\frac{7}{20736}[\epsilon_6^{(3)}, \epsilon_6^{(4)}]$ at degree 12, $\frac{7}{4147200}([\epsilon_6^{(1)}, \epsilon_8^{(6)}] - [\epsilon_6^{(2)}, \epsilon_8^{(5)}] + [\epsilon_6^{(3)}, \epsilon_8^{(4)}] - [\epsilon_6^{(4)}, \epsilon_8^{(3)}])$ at degree 14 and $-\frac{1}{26127360}([\epsilon_8^{(1)}, \epsilon_8^{(6)}] - [\epsilon_8^{(2)}, \epsilon_8^{(5)}] + [\epsilon_8^{(3)}, \epsilon_8^{(4)}])$ at degree 16.

iteration of the projector t^d to lowest-weight vectors),

$$
\begin{aligned}
[z_3,\epsilon_k]^{\{3\}} &= \frac{3\mathrm{BF}_4\mathrm{BF}_{k-2}}{\mathrm{BF}_k}\left\{-\frac{(k-3)}{(k-1)}\,t^2(\epsilon_4,t^3(\epsilon_4,\epsilon_{k-2}))+\frac{(k-2)}{k}\,t^3(\epsilon_4,t^2(\epsilon_4,\epsilon_{k-2}))\right\} \\
&\quad+\frac{1}{(k-1)\mathrm{BF}_k}\sum_{\ell=6}^{k-4}(\ell-1)\mathrm{BF}_\ell\mathrm{BF}_{k+2-\ell} \\
&\qquad\times\left\{-\frac{2(k-\ell+1)}{(k-\ell+2)}\,t^2(\epsilon_\ell,t^3(\epsilon_4,\epsilon_{k+2-\ell}))+\frac{\ell-2}{k}\,t^3(\epsilon_\ell,t^2(\epsilon_4,\epsilon_{k+2-\ell}))\right\}
\end{aligned}
\tag{7.19}
$$

and

$$
\begin{aligned}
[z_5,\epsilon_k]^{\{3\}} &= \frac{\mathrm{BF}_{k+2}\mathrm{BF}_2^3}{2\mathrm{BF}_4\mathrm{BF}_k}\,t^4(\epsilon_{k+2},t^3(\epsilon_4,\epsilon_4)) \\
&\quad+\frac{5\mathrm{BF}_6\mathrm{BF}_{k-2}}{\mathrm{BF}_k}\left\{-\frac{(k-5)}{(k-1)}\,t^2(\epsilon_6,t^5(\epsilon_6,\epsilon_{k-2}))+\frac{2(k-3)(k-4)}{k(k-1)}\,t^3(\epsilon_6,t^4(\epsilon_6,\epsilon_{k-2}))\right. \\
&\qquad\left.-\frac{2(k-2)(k-3)}{k(k+1)}\,t^4(\epsilon_6,t^3(\epsilon_6,\epsilon_{k-2}))+\frac{(k-2)}{(k+2)}\,t^5(\epsilon_6,t^2(\epsilon_6,\epsilon_{k-2}))\right\} \\
&\quad+\mathrm{BF}_4\left\{-\frac{12(k-3)}{k(k-1)}\,t^2(\epsilon_4,t^5(\epsilon_6,\epsilon_k))+\frac{36(k-2)}{k^2(k+1)}\,t^3(\epsilon_4,t^4(\epsilon_6,\epsilon_k))\right. \\
&\qquad-\frac{24}{k(k+1)(k+2)}\,t^4(\epsilon_4,t^3(\epsilon_6,\epsilon_k))-\frac{9(k-2)}{5k}\,t^3(\epsilon_k,t^4(\epsilon_4,\epsilon_6)) \\
&\qquad\left.-\frac{2(k-2)(k-3)}{k(k+1)}\,t^4(\epsilon_k,t^3(\epsilon_4,\epsilon_6))-\frac{(k-2)(k-3)(k-4)}{k(k+1)(k+2)}t^5(\epsilon_k,t^2(\epsilon_4,\epsilon_6))\right\} \\
&\quad+\frac{1}{(k-1)\mathrm{BF}_k}\sum_{\ell=8}^{k-4}(\ell-1)\mathrm{BF}_\ell\mathrm{BF}_{k+4-\ell}\left\{-\frac{4(k-\ell+1)}{(k-\ell+4)}\,t^2(\epsilon_\ell,t^5(\epsilon_6,\epsilon_{k+4-\ell}))\right. \\
&\qquad+\frac{6(\ell-2)(k-\ell+2)(k-\ell+3)}{k(k-\ell+4)(k-\ell+5)}\,t^3(\epsilon_\ell,t^4(\epsilon_6,\epsilon_{k+4-\ell})) \\
&\qquad-\frac{4(\ell-3)(\ell-2)(k-\ell+3)}{k(k+1)(k-\ell+6)}\,t^4(\epsilon_\ell,t^3(\epsilon_6,\epsilon_{k+4-\ell})) \\
&\qquad\left.+\frac{(\ell-2)(\ell-3)(\ell-4)}{k(k+1)(k+2)}\,t^5(\epsilon_\ell,t^2(\epsilon_6,\epsilon_{k+4-\ell}))\right\}.
\end{aligned}
\tag{7.20}
$$

The remaining brackets $[z_w,\epsilon_k]^{\{3\}}$ at degree ≤ 20 are given by

$$
\begin{aligned}
[z_7,\epsilon_4]^{\{3\}} &= \frac{\mathrm{BF}_8\mathrm{BF}_2^2}{\mathrm{BF}_6}\,t^6(\epsilon_8,t^3(\epsilon_4,\epsilon_6))+\frac{\mathrm{BF}_6\mathrm{BF}_2^2}{2\mathrm{BF}_4}\,t^4(\epsilon_6,t^5(\epsilon_6,\epsilon_6)) \\
&\quad-\mathrm{BF}_6\left\{\frac{15}{14}\,t^3(\epsilon_4,t^6(\epsilon_6,\epsilon_8))+\frac{5}{14}\,t^4(\epsilon_4,t^5(\epsilon_6,\epsilon_8))\right. \\
&\qquad\left.+\frac{5}{7}\,t^5(\epsilon_4,t^4(\epsilon_6,\epsilon_8))+\frac{3}{28}\,t^6(\epsilon_4,t^3(\epsilon_6,\epsilon_8))\right\},
\end{aligned}
\tag{7.21}
$$

$$[z_7,\epsilon_6]^{\{3\}} = \frac{\mathrm{BF}_{10}\mathrm{BF}_4\mathrm{BF}_2^2}{\mathrm{BF}_6^2}\, t^6(\epsilon_{10},t^3(\epsilon_4,\epsilon_6)) + \frac{\mathrm{BF}_8\mathrm{BF}_2^2}{2\mathrm{BF}_6}\, t^4(\epsilon_8,t^5(\epsilon_6,\epsilon_6))$$
$$- \frac{\mathrm{BF}_4\mathrm{BF}_8}{\mathrm{BF}_6}\bigg\{ \frac{5}{2}\, t^5(\epsilon_8,t^4(\epsilon_4,\epsilon_8)) + \frac{7}{2}\, t^6(\epsilon_8,t^3(\epsilon_4,\epsilon_8)) + \frac{14}{5}\, t^7(\epsilon_8,t^2(\epsilon_4,\epsilon_8)) \bigg\}$$
$$- \mathrm{BF}_6\bigg\{ \frac{10}{7}\, t^3(\epsilon_6,t^6(\epsilon_6,\epsilon_8)) + \frac{50}{49}\, t^4(\epsilon_6,t^5(\epsilon_6,\epsilon_8))$$
$$+ \frac{25}{84}\, t^5(\epsilon_6,t^4(\epsilon_6,\epsilon_8)) + \frac{1}{42}\, t^6(\epsilon_6,t^3(\epsilon_6,\epsilon_8)) \bigg\}.$$

7.4.3 Exact results for σ_3 and z_3

Once the complete set of highest-weight vectors for a given σ_w is available, then the recursion (7.10) determines all-degree expressions for both $\sigma_w^{\{2\}}, \sigma_w^{\{3\}}, \ldots, \sigma_w^{\{w\}}$ and $[z_w,\epsilon_k]^{\{2\}}, [z_w,\epsilon_k]^{\{3\}}, \ldots, [z_w,\epsilon_k]^{\{w+1\}}$. With the highest-weight vectors for $\sigma_3,\sigma_5,\sigma_7$ noted in section 7.1, there is no obstruction to algorithmically assembling the exact results for the expansions of σ_w and $[z_w,\epsilon_k]$ at $w\leq 7$.

We shall here display the exact results for σ_3 and $[z_3,\epsilon_k]$ which terminate with modular depth three and four, respectively. The all-order expansion of σ_3 is given by,

$$\sigma_3 = -\frac{1}{2}\epsilon_4^{(2)} + z_3 + \frac{1}{480}[\epsilon_4,\epsilon_4^{(1)}] + \sum_{k=6}^{\infty} \mathrm{BF}_k \bigg([\epsilon_4^{(1)},\epsilon_k] - \frac{[\epsilon_4,\epsilon_k^{(1)}]}{k-2} \bigg)$$
$$+ \sum_{m=4}^{\infty}\sum_{r=6}^{\infty} \frac{(m-1)\mathrm{BF}_m\mathrm{BF}_r}{m+r-2}\big[\epsilon_m,[\epsilon_4,\epsilon_r]\big]\,, \tag{7.22}$$

where the second line is obtained by solving (7.11) at $m=w=3$ for $\sigma_3^{\{3\}}$ with the expression for $\sigma_3^{\{2\}}$ determined by the first line. The action of the arithmetic part z_3 on a,b can be found in (5.47). The expression for $[z_3,\epsilon_k]$ resulting from $[N,\sigma_3]=0$ can be assembled by combining $[z_3,\epsilon_k]^{\{2\}} = \frac{\mathrm{BF}_{k+2}}{\mathrm{BF}_k} t^4(\epsilon_4,\epsilon_{k+2})$ from (7.15) with the expression (7.19) for $[z_3,\epsilon_k]^{\{3\}}$ and the degree-$(2w+k)$ parts of

$$\sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k[z_3,\epsilon_k]^{\{4\}} = \sum_{k=4}^{\infty}(k-1)\mathrm{BF}_k\sum_{m=4}^{\infty}\sum_{r=6}^{\infty}\frac{(m-1)\mathrm{BF}_m\mathrm{BF}_r}{(m+r-2)}[\epsilon_k,[\epsilon_m,[\epsilon_4,\epsilon_r]]] \tag{7.23}$$

which follows from (7.16) at $w=3$. The lowest-degree examples of $[z_3,\epsilon_k]^{\{4\}}$ occur in

$$[z_3,\epsilon_{12}] = \frac{\mathrm{BF}_{14}}{\mathrm{BF}_{12}}t^4(\epsilon_4,\epsilon_{14}) + \frac{\mathrm{BF}_4\mathrm{BF}_{10}}{\mathrm{BF}_{12}}\bigg\{ -\frac{27}{11}t^2(\epsilon_4,t^3(\epsilon_4,\epsilon_{10})) + \frac{5}{2}t^3(\epsilon_4,t^2(\epsilon_4,\epsilon_{10})) \bigg\}$$
$$+ \frac{\mathrm{BF}_6\mathrm{BF}_8}{\mathrm{BF}_{12}}\bigg\{ -\frac{35}{44}t^2(\epsilon_6,t^3(\epsilon_4,\epsilon_8)) + \frac{5}{33}t^3(\epsilon_6,t^2(\epsilon_4,\epsilon_8))$$
$$- \frac{35}{33}t^2(\epsilon_8,t^3(\epsilon_4,\epsilon_6)) + \frac{7}{22}t^3(\epsilon_8,t^2(\epsilon_4,\epsilon_6)) \bigg\}$$
$$+ \frac{9\mathrm{BF}_4^2\mathrm{BF}_6}{88\mathrm{BF}_{12}}[\epsilon_4,[\epsilon_4,[\epsilon_4,\epsilon_6]]]$$

as well as

$$
\begin{aligned}
[z_3, \epsilon_{14}] &= \frac{\mathrm{BF}_{16}}{\mathrm{BF}_{14}} t^4(\epsilon_4, \epsilon_{16}) + \frac{\mathrm{BF}_4 \mathrm{BF}_{12}}{\mathrm{BF}_{14}} \bigg\{ \frac{18}{7} t^3(\epsilon_4, t^2(\epsilon_4, \epsilon_{12})) - \frac{33}{13} t^2(\epsilon_4, t^3(\epsilon_4, \epsilon_{12})) \bigg\} \\
&\quad + \frac{\mathrm{BF}_6 \mathrm{BF}_{10}}{\mathrm{BF}_{14}} \bigg\{ \frac{10}{91} t^3(\epsilon_6, t^2(\epsilon_4, \epsilon_{10})) - \frac{9}{13} t^2(\epsilon_6, t^3(\epsilon_4, \epsilon_{10})) \\
&\qquad\qquad + \frac{36}{91} t^3(\epsilon_{10}, t^2(\epsilon_4, \epsilon_6)) - \frac{15}{13} t^2(\epsilon_{10}, t^3(\epsilon_4, \epsilon_6)) \bigg\} \\
&\quad + \frac{\mathrm{BF}_8^2}{\mathrm{BF}_{14}} \bigg\{ \frac{3}{13} t^3(\epsilon_8, t^2(\epsilon_4, \epsilon_8)) - \frac{49}{52} t^2(\epsilon_8, t^3(\epsilon_4, \epsilon_8)) \bigg\} \\
&\quad + \frac{9\mathrm{BF}_4^2 \mathrm{BF}_8}{130\mathrm{BF}_{14}} [\epsilon_4, [\epsilon_4, [\epsilon_4, \epsilon_8]]] + \frac{27\mathrm{BF}_4 \mathrm{BF}_6^2}{104\mathrm{BF}_{14}} [\epsilon_4, [\epsilon_6, [\epsilon_4, \epsilon_6]]] \, ,
\end{aligned}
$$

also see appendix E.1 of [8] for $[z_3, \epsilon_k]$ at $k = 4, 6, 8, 10$.

7.4.4 Highest-weight vectors at modular depth three

While a comprehensive study of highest-weight vector contributions to $\sigma_w^{\{m \geq 3\}}$ is left for the future, their instances at $w \leq 11$ are accessible from the ancillary files of [8]. The simplest highest-weight vector at modular depth three occurs in the expansion (5.49) of σ_7 at degree 12 and can be compactly written as $-\frac{661}{14400} s^3(\epsilon_4, t^3(\epsilon_4, \epsilon_4))$ through the combination (7.7) of s^d and t^d operations. This shorthand also streamlines the expansions of σ_9, σ_{11} to

$$
\begin{aligned}
\sigma_9 &= -\frac{\epsilon_{10}^{(8)}}{8!} + \frac{5s^3(\epsilon_4, \epsilon_8)}{18} + \frac{7s^3(\epsilon_6, \epsilon_6)}{72} + \frac{s^5(\epsilon_4, \epsilon_{10})}{720} - \frac{7s^5(\epsilon_6, \epsilon_8)}{1440} \\
&\quad + \frac{34921 s^2(\epsilon_4, t^4(\epsilon_4, \epsilon_6))}{1134000} + \frac{2587 s^3(\epsilon_4, t^3(\epsilon_4, \epsilon_6))}{37800} - \frac{529 s^4(\epsilon_4, t^2(\epsilon_4, \epsilon_6))}{14400} \\
&\quad - \frac{s^7(\epsilon_6, \epsilon_{10})}{30240} + \frac{s^7(\epsilon_8, \epsilon_8)}{12096} + \frac{s^5(\epsilon_4, t^3(\epsilon_4, \epsilon_8))}{2592} + \frac{7s^5(\epsilon_4, t^3(\epsilon_6, \epsilon_6))}{51840} \\
&\quad - \frac{34921 s^4(\epsilon_6, t^4(\epsilon_6, \epsilon_4))}{47628000} - \frac{2587 s^5(\epsilon_6, t^3(\epsilon_6, \epsilon_4))}{1587600} + \frac{529 s^6(\epsilon_6, t^2(\epsilon_6, \epsilon_4))}{604800} \\
&\quad \frac{149 s^3(\epsilon_4, t^3(\epsilon_4, t^3(\epsilon_4, \epsilon_4)))}{13824} - \frac{149 s^4(\epsilon_4, t^2(\epsilon_4, t^3(\epsilon_4, \epsilon_4)))}{69120} + \ldots \\
\sigma_{11} &= -\frac{\epsilon_{12}^{(10)}}{10!} + \frac{11 s^3(\epsilon_4, \epsilon_{10})}{40} + \frac{11 s^3(\epsilon_6, \epsilon_8)}{60} + \frac{242407 s^2(\epsilon_4, t^2(\epsilon_4, \epsilon_6))}{14735232} + \frac{s^5(\epsilon_4, \epsilon_{12})}{720} \\
&\quad - \frac{s^5(\epsilon_6, \epsilon_{10})}{216} - \frac{7s^5(\epsilon_8, \epsilon_8)}{4320} + \frac{11090423 s^2(\epsilon_4, t^4(\epsilon_4, \epsilon_8))}{309439872} + \frac{3197 s^3(\epsilon_4, t^3(\epsilon_4, \epsilon_8))}{57600} \\
&\quad - \frac{2983 s^4(\epsilon_4, t^2(\epsilon_4, \epsilon_8))}{86400} + \frac{148753 s^3(\epsilon_4, t^3(\epsilon_6, \epsilon_6))}{7367616} + \frac{490853 s^3(\epsilon_6, t^3(\epsilon_6, \epsilon_4))}{17191104} \\
&\quad + \frac{156805 s^4(\epsilon_6, t^2(\epsilon_6, \epsilon_4))}{14735232} + c\, s^2(\epsilon_4, t^2(\epsilon_4, t^3(\epsilon_4, \epsilon_4))) + \ldots \, ,
\end{aligned}
\tag{7.24}
$$

where the ellipsis refers to all contributions of degree ≥ 18, and the coefficient $c \in \mathbb{Q}$ of the first modular-depth-four contribution to σ_{11} in the last line has not yet been computed. It is, however, a highest weight vector and entirely fixed by our construction. Note that the $s^{d_2}(\epsilon_{k_3}, t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2}))$ only furnish highest-weight vectors if $d_2 \leq \min(k_3, r)$, where $r = k_1 + k_2 - 2d_1 + 2$. Accordingly, all the terms $s^{d_2}(\epsilon_{k_3}, t^{d_1}(\epsilon_{k_1}, \epsilon_{k_2}))$ of modular depth three in (7.24) are highest-weight vectors with the exception of the contributions $s^5(\epsilon_4, t^3(\epsilon_4, \epsilon_8))$ and $s^5(\epsilon_4, t^3(\epsilon_6, \epsilon_6))$ to σ_9. The ancillary files of [8] provide all contributions to $\sigma_w^{\{m\leq 3\}}$ at degree ≤ 20 in machine-readable form which determines all the highest-weight vectors of $\sigma_9^{\{3\}}$ and $\sigma_{11}^{\{3\}}$.

A Deriving the topological map from the sphere to the torus

The goal of this appendix is to derive the explicit form of the map (5.29) and (5.30) between the generators x, y and a, b of the fundamental groups in genus zero and genus one, respectively. Our derivation will be based on a formulation of the zeta generators in terms of Knizhnik–Zamolodchikov (KZ) connections in genus zero and Knizhnik–Zamolodchikov–Bernard (KZB) connections in genus one. The form of the KZ connection obtained from the degeneration limit of the KZB connection then relates the generators x, y of the fundamental group of the thrice punctured sphere to the generators a, b of the fundamental group of the once-punctured torus.

A.1 Zeta generators in terms of the KZ connection

In this appendix we assume the conjecture that the surjection from motivic to real MZVs is an isomorphism, and thus identify the motivic version $\Phi^{\mathfrak{m}}(x, y)$ of the modified Drinfeld associator with $\Phi(x, y)$ as defined in (3.42). We will systematically assume that $\Phi(x, y)$ is written in the semi-canonical basis defined in section 3.5, and use the notation

$$g_w = \Phi(x, y)|_{\zeta_w} \tag{A.1}$$

for the canonical polynomial g_w that then appears in Φ with coefficient ζ_w for odd $w \geq 3$ (see Definition 3.3.4). The power series $\Phi(x, y)$ in (3.42) can be obtained as the path-ordered exponential of the modified KZ connection J defined by[17]

$$\begin{aligned} J(x, y; z) &= \left(\frac{x}{z} + \frac{y}{1-z}\right) dz\,, \qquad z \in \mathbb{C} \setminus \{0, 1\}\,, \\ \Phi(x, y) &= \mathrm{Pexp}\left(\int_0^1 J(x, y; z)\right), \\ g_w(x, y) &= \Phi(x, y)\,\big|_{\zeta_w} = \mathrm{Pexp}\left(\int_0^1 \left[\frac{x}{z} + \frac{y}{1-z}\right] dz\right)\big|_{\zeta_w}\,, \end{aligned} \tag{A.2}$$

[17]The connection $J(x, y; z)$ differs from the classical KZ connection $J_{\mathrm{KZ}}(x, y; z) = \left(\frac{x}{z} + \frac{y}{z-1}\right) dz$ by changing y to $-y$, corresponding to the relation $\Phi(x, y) = \Phi_{\mathrm{KZ}}(x, -y)$ between the power series Φ and the classical Drinfeld associator (3.41) obtained by path-ordered integration of J_{KZ}.

where the iterated integration is taken over the simplex $0 < z_1 < \cdots < z_r < 1$, and the convention for expanding path-ordered exponentials is

$$\text{Pexp}\left(\int_0^1 J(z)\right) = 1 + \sum_{r=1}^{\infty} \int_0^1 J(z_r) \int_0^{z_r} J(z_{r-1}) \cdots \int_0^{z_3} J(z_2) \int_0^{z_2} J(z_1)\,. \tag{A.3}$$

The endpoint divergences in (A.3) are understood to be regularized by passing to shuffle-regularized versions (2.3) of the MZVs in the expansion of $\Phi(x, y)$.

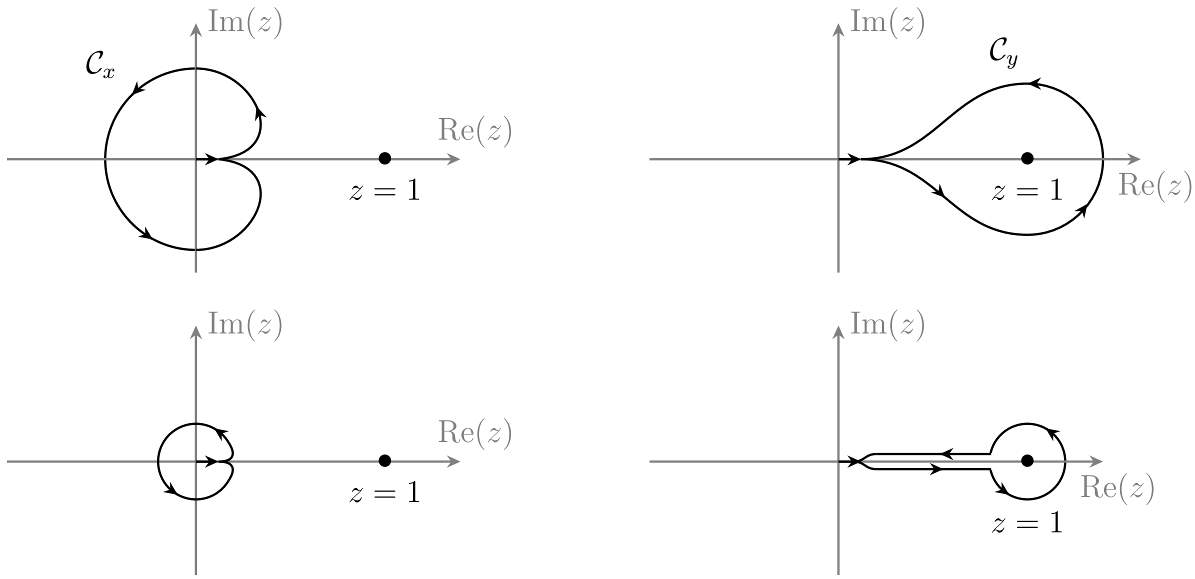

Figure 3: *The loops $\mathcal{C}_x$ and $\mathcal{C}_y$ around $z = 0$ and $z = 1$ anchored at the origin (upper half) and their homotopy deformation to infinitesimal circles along with straight paths between zero and one in case of $\mathcal{C}_y$ (lower half) [71]. Strictly speaking, all the contours start and end at the tangential base point from 0 to 1 as indicated by the arrows at the origin pointing along the positive real axis. The straight line portions of the path in the lower-right panel should be viewed as running along the real axis between 0 and 1; they have been slightly separated for visual convenience.*

The zeta generators in genus zero are given by the Ihara derivations D_{g_w} associated to the polynomials g_w, which act on the free Lie algebra Lie$[x, y]$ via

$$D_{g_w}(x) = 0\,, \qquad D_{g_w}(y) = [y, g_w(x, y)]\,; \tag{A.4}$$

they can be interpreted as the coefficient of ζ_w in the holonomies of $J(x, y; z)$ w.r.t. the loops around $z = 0$ and $z = 1$, respectively. More specifically, (A.4) extracts the *linearized* monodromy of the loops $\mathcal{C}_x$ and $\mathcal{C}_y$ around $z = 0$ and $z = 1$ anchored at the origin as drawn in Figure 3, where only the first power of $2\pi i$ is retained:

$$D_{g_w}(x) = -\text{Pexp}\left(\int_{\mathcal{C}_x} J(x, y; z)\right)\Big|_{2\pi i \zeta_w}\,,$$

$$D_{g_w}(y) = -\text{Pexp}\Big(\int_{\mathcal{C}_y} J(x,y;z) \Big) \big|_{2\pi i \zeta_w} \tag{A.5}$$

Equivalence to (A.4) can be seen as follows:

- The path-ordered exponentials of $J(x,y;z)$ associated with the infinitesimal circles around 0 and 1 in counter-clockwise orientation are given by $e^{2\pi i x}$ and $e^{-2\pi i y}$, respectively.
- Since $\mathcal{C}_x$ is homotopic to an infinitesimal circle around $z=0$, we have

  $$\text{Pexp}\Big(\int_{\mathcal{C}_x} J(x,y;z) \Big) = e^{2\pi i x} \tag{A.6}$$

  and does not contain any odd Riemann zeta values, thereby reproducing $D_{g_w}(x) = 0$.
- The path $\mathcal{C}_y$ is homotopic to the composition of the path $(0,1)$ followed by an infinitesimal circle around $z=1$ and the inverse path $(1,0)$ as seen in the lower-right panel of Figure 3. Hence, the path-ordered exponential can be decomposed into

  $$\text{Pexp}\Big(\int_{\mathcal{C}_y} J(x,y;z) \Big) = \Phi(x,y)^{-1} e^{-2\pi i y} \Phi(x,y) \,. \tag{A.7}$$

  By the conventions (A.3) for path-ordered exponentials, the last segment $(1,0)$ of the deformed path $\mathcal{C}_y$ translates into the leftmost factor $\Phi(x,y)^{-1}$.
- Extracting the coefficient of ζ_w from (A.7) leads to

  $$\text{Pexp}\Big(\int_{\mathcal{C}_y} J(x,y;z) \Big) \big|_{\zeta_w} = e^{-2\pi i y} g_w(x,y) - g_w(x,y) e^{-2\pi i y} \tag{A.8}$$

  which upon linearization in $2\pi i$ reduces to $-2\pi i [y, g_w(x,y)]$ and reproduces the action of D_{g_w} on y in (A.4).

We emphasize that it will be the formulation (A.5) of zeta generators in terms of linearized monodromies which generalizes from genus zero to genus one.

A.2 Degenerating the KZB connection

In the same way as the (modified) KZ connection (A.2) can be used to generate multiple polylogarithms in genus zero, the Brown–Levin formulation of elliptic polylogarithms in genus one [86] is based on the KZB connection

$$J_{\text{KZB}}(A,B;z|\tau) = \text{ad}_B F(z, \text{ad}_B|\tau) A \, dz \,, \qquad F(z,\alpha|\tau) = \frac{\theta_1'(0|\tau)\theta_1(z+\alpha|\tau)}{\theta_1(z|\tau)\theta_1(\alpha|\tau)} \,, \tag{A.9}$$

$$\theta_1(z|\tau) = 2q^{1/8} \sin(\pi z) \prod_{n=1}^{\infty} (1-q^n)(1-e^{2\pi i z} q^n)(1-e^{-2\pi i z} q^n) \,, \qquad q = e^{2\pi i \tau} \,,$$

where $F(z,\alpha|\tau)$ is known as the Kronecker–Eisenstein series. The modular parameter $\tau \in \mathbb{H}$ of the torus takes values in the upper half plane $\mathbb{H} = \{\tau \in \mathbb{C}\,,\ \mathrm{Im}\,\tau > 0\}$, and $z, \alpha \in \mathbb{C}$ live on the universal cover of the torus $\mathbb{C}/(\mathbb{Z}+\tau\mathbb{Z})$. The KZB connection $J_{\rm KZB}$ depends on non-commutative indeterminates A, B, and the adjoint actions of B in $\mathrm{ad}_B F(z, \mathrm{ad}_B|\tau)$ are performed after series expansion in the second argument of F. Note that the elliptic associators of [72, 20, 79] are obtained from (regularized) path-ordered exponentials of (A.9), integrated over the homology cycles of the torus.

The degeneration $\tau \to i\infty$ of the Kronecker–Eisenstein series and its expansion coefficients w.r.t. the second argument $\alpha = \mathrm{ad}_B$ is well-known to yield [87]

$$\lim_{\tau \to i\infty} F(z,\alpha|\tau) = \frac{1}{\alpha} + \pi\cot(\pi z) - 2\sum_{n=1}^{\infty} \alpha^{2n-1}\zeta_{2n}\,. \tag{A.10}$$

The limit $\tau \to i\infty$ degenerates the torus to a nodal sphere. In the coordinate $\sigma = e^{2\pi i z}$ of the nodal sphere, the pinched homology cycle of the degenerate torus translates into the identification of the points $\sigma = 0$ with $\sigma = \infty$. Based on $dz = \frac{d\sigma}{2\pi i \sigma}$ and (A.10), the degeneration of the KZB connection (A.9) is readily found to be

$$\lim_{\tau\to i\infty} J_{\rm KZB}(A,B;z|\tau) = \left\{ A + 2\pi i \left(-\frac{1}{2} + \frac{\sigma}{\sigma-1} \right) [B,A] + \sum_{n=1}^{\infty} (2\pi i)^{2n} \frac{\mathrm{B}_{2n}}{(2n)!} \mathrm{ad}_B^{2n} A \right\} \frac{d\sigma}{2\pi i \sigma}\,. \tag{A.11}$$

In order to make contact with the images t_{01} and t_{12} in (5.30) of the genus-zero generators x, y, we redefine the non-commutative A, B in (A.9) in terms of the generators a, b introduced in section 5.1

$$A = -2\pi i a\,, \qquad B = \frac{b}{2\pi i} \tag{A.12}$$

and obtain the (modified) KZ connection (A.2) at $x = t_{01}$ and $y = -t_{12}$ from the degeneration (A.11),

$$\lim_{\tau\to i\infty} J_{\rm KZB}(A,B;z|\tau) = \left(\frac{t_{01}}{\sigma} + \frac{-t_{12}}{1-\sigma} \right) d\sigma = J(t_{01}, -t_{12}; \sigma)\,. \tag{A.13}$$

A.3 Link between genus zero and genus one

The non-commutative arguments t_{01}, t_{12} obtained in the comparison (A.13) of KZ and KZB connections do not yet line up with (5.29) and differ by a swap of x and y. This can be fixed by an additional change of coordinates to $\eta = 1-\sigma$ in the degeneration of the KZB connection which is in fact necessary to map the origin $z=0$ of the torus to the origin $\eta = 0$ of the nodal sphere (as opposed to $\sigma = 1$). In this way, the homotopy deformation of the contour $\mathcal{C}_y$ of Figure 3 producing the action of zeta generators in genus zero is the image of the A-cycle of the torus $z \in (0,1)$ under the change of variables from z via $\sigma = e^{2\pi i z}$ to $\eta = 1-\sigma$, see Figure 4. Similar homotopy deformations of paths together with the degeneration (A.13) of the KZB connection were used by Enriquez to express the limit $\tau \to i\infty$ of elliptic associators in terms of $\Phi_{\rm KZ}$ [73].

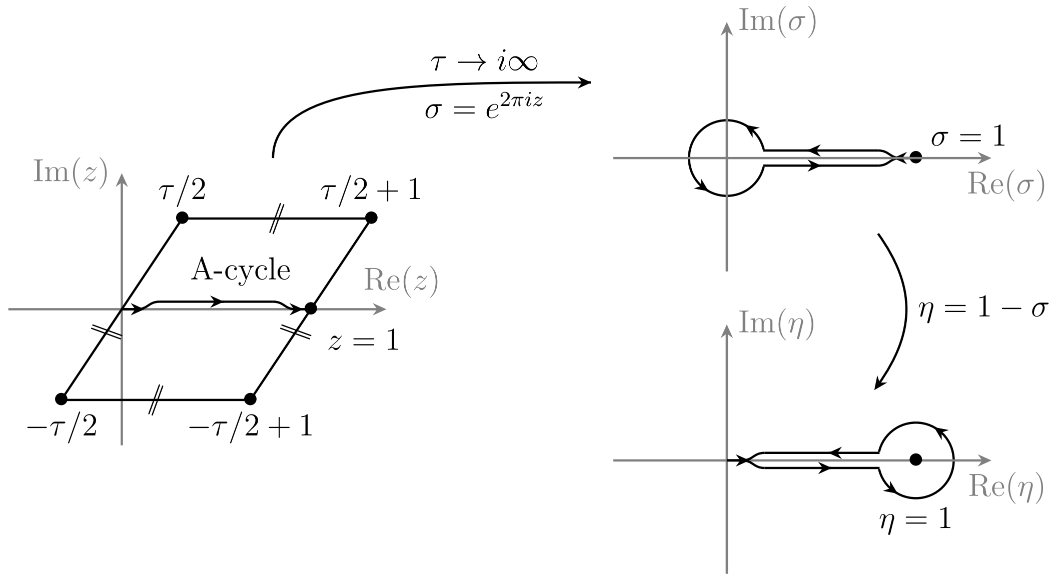

Figure 4: *The degeneration $\tau \to i\infty$ of the torus with coordinate z (left panel) yields a nodal sphere, where the image of the A-cycle connecting $z=0$ with $z=1$ is drawn in two different coordinates σ and η (right panel). The image of the A-cycle in the η coordinate (lower-right panel) matches the deformation of the loop $\mathcal{C}_y$ around $z=1$ in Figure 3. Similar to Figure 3, the straight line portions of all the paths should be viewed as running along the real axis between 0 and 1; they have been slightly separated for visual convenience.*

With the degenerate KZB connection in the coordinate $\eta = 1-\sigma$

$$\lim_{\tau\to i\infty} J_{\rm KZB}(A,B;z|\tau) = \left(\frac{t_{12}}{\eta} + \frac{-t_{01}}{1-\eta}\right) d\eta = J(t_{12},-t_{01};\eta)\,, \tag{A.14}$$

we obtain the factor

$$g_w(t_{12},-t_{01}) = \text{Pexp}\bigg(\int_0^1 \left[\frac{t_{12}}{\eta} + \frac{-t_{01}}{1-\eta}\right] d\eta\bigg)\,\Big|_{\zeta_w} \tag{A.15}$$

in the action (5.42) of genus-one zeta generators on t_{01}, in direct analogy with (A.2) in genus zero. Moreover, the realization (A.5) of $D_{g_w}(y)$ in genus zero generalizes to

$$\begin{aligned}\tau_w(t_{01}) &= -\text{Pexp}\bigg(\int_{\mathcal{C}_y} \left[\frac{t_{12}}{\eta} + \frac{-t_{01}}{1-\eta}\right] d\eta\bigg)\,\Big|_{2\pi i\zeta_w}\,, \\ &= -\lim_{\tau\to i\infty} \text{Pexp}\bigg(\int_0^1 J_{\rm KZB}(A,B;z|\tau)\bigg)\,\Big|_{2\pi i \zeta_w}\,,\end{aligned} \tag{A.16}$$

i.e. the interpretation as a linearized monodromy passes through from genus zero to genus one. The loop $\mathcal{C}_y$ anchored at the origin of the sphere around the point $\eta = 1$ descends from the A-cycle $z \in (0,1)$ of the torus. The other part $\tau_w(t_{12}) = 0$ of the action (5.42) of genus-one zeta generators in turn follows from a loop around the origin of both the sphere ($\eta = 0$) and the torus ($z = 0$) which can be contracted to an infinitesimal circle and does not produce any odd zeta values through its periods, see (A.6).

In summary, this appendix derived the close analogy between the actions (A.4) and (5.42) of zeta generators in genus zero and one and justified the morphism (5.29) by comparing (i) the underlying connections of KZ- and KZB-type in the degeneration of the torus to a nodal sphere and (ii) integration contours on the respective surfaces (loops around marked points and the pinched homology cycle of the degenerate torus).

References

[1] F. Brown, "Polylogarithmes multiples uniformes en une variable," *C. R. Acad. Sci. Paris* **Ser. I 338** (2004) 527–532.

[2] J. Broedel, M. Sprenger, and A. Torres Orjuela, "Towards single-valued polylogarithms in two variables for the seven-point remainder function in multi-Regge-kinematics," *Nucl. Phys. B* **915** (2017) 394–413, arXiv:1606.08411 [hep-th].

[3] V. Del Duca, S. Druc, J. Drummond, C. Duhr, F. Dulat, R. Marzucca, G. Papathanasiou, and B. Verbeek, "Multi-Regge kinematics and the moduli space of Riemann spheres with marked points," *JHEP* **08** (2016) 152, arXiv:1606.08807 [hep-th].

[4] H. Frost, M. Hidding, D. Kamlesh, C. Rodriguez, O. Schlotterer, and B. Verbeek, "Motivic coaction and single-valued map of polylogarithms from zeta generators," arXiv:2312.00697 [hep-th].

[5] F. Brown, "A class of non-holomorphic modular forms I," *Res. Math. Sci.* **5** (2018) 5:7, arXiv:1707.01230 [math.NT].

[6] F. Brown, "A class of non-holomorphic modular forms II : equivariant iterated Eisenstein integrals," *Forum of Mathematics, Sigma* **8** (2020) 1, arXiv:1708.03354 [math.NT].

[7] D. Dorigoni, M. Doroudiani, J. Drewitt, M. Hidding, A. Kleinschmidt, N. Matthes, O. Schlotterer, and B. Verbeek, "Modular graph forms from equivariant iterated Eisenstein integrals," *JHEP* **12** (2022) 162, arXiv:2209.06772 [hep-th].

[8] D. Dorigoni, M. Doroudiani, J. Drewitt, M. Hidding, A. Kleinschmidt, O. Schlotterer, L. Schneps, and B. Verbeek, "Non-holomorphic modular forms from zeta generators," arXiv:2403.14816 [hep-th].

[9] E. D'Hoker, M. B. Green, Ö. Gürdogan, and P. Vanhove, "Modular graph functions," *Commun. Num. Theor. Phys.* **11** (2017) 165–218, arXiv:1512.06779 [hep-th].

[10] E. D'Hoker and M. B. Green, "Identities between modular graph forms," *J. Number Theory* **189** (2018) 25–80, arXiv:1603.00839 [hep-th].

[11] J. E. Gerken, "Modular Graph Forms and Scattering Amplitudes in String Theory," arXiv:2011.08647 [hep-th].

[12] N. Berkovits, E. D'Hoker, M. B. Green, H. Johansson, and O. Schlotterer, "Snowmass White Paper: String Perturbation Theory," in *2022 Snowmass Summer Study*. 3, 2022. arXiv:2203.09099 [hep-th].

[13] E. D'Hoker and J. Kaidi, "Lectures on modular forms and strings," arXiv:2208.07242 [hep-th].

[14] F. Brown, "On the decomposition of motivic multiple zeta values," in *Galois-Teichmüller theory and arithmetic geometry*, vol. 63 of *Adv. Stud. Pure Math.*, pp. 31–58. Math. Soc. Japan, Tokyo, 2012. arXiv:1102.1310 [math.NT].

[15] F. Brown, "Mixed Tate motives over $\mathbb{Z}$," *Ann. Math.* **175** (2012) no. 2, 949–976, arXiv:1102.1312 [math.AG].

[16] M. Levine, "Tate motives and the vanishing conjectures for algebraic K-theory," in *Algebraic K-theory and algebraic topology (Lake Louise, AB, 1991)*, vol. 407 of *NATO Adv. Sci. Inst. Ser. C: Math. Phys. Sci.*, pp. 167–188. Kluwer Acad. Publ., Dordrecht, 1993.

[17] L. Schneps, "Dual-depth adapted irreducible formal multizeta values," *Math. Scand.* **113** (2013) no. 1, 53–62.

[18] V. Drinfeld, "Quasi Hopf algebras," *Leningrad Math.* **J. 1** (1989) 1419–1457.

[19] V. Drinfeld, "On quasitriangular quasi-Hopf algebras and on a group that is closely connected with $\mathrm{Gal}(\bar{\mathbb{Q}}/\mathbb{Q})$," *Leningrad Math.* **J. 2 (4)** (1991) 829–860.

[20] B. Enriquez, "Elliptic associators," *Selecta Math. (N.S.)* **20** (2014) no. 2, 491–584, arXiv:1003.1012 [math.QA].

[21] R. Hain and M. Matsumoto, "Universal mixed elliptic motives," *Journal of the Institute of Mathematics of Jussieu* **19** (2020) no. 3, 663–766, arXiv:1512.03975 [math.AG].

[22] J. Écalle, "The flexion structure and dimorphy: flexion units, singulators, generators, and the enumeration of multizeta irreducibles," *CRM Series* **12** (2011) 27–211.

[23] L. Schneps, "Elliptic double shuffle, Grothendieck-Teichmüller and mould theory," *Ann. Math. Québec* **44(2)** (2020) 261–289, arXiv:1506.09050 [math.NT].

[24] Y. Ihara, "Some arithmetic aspects of Galois actions in the pro-p fundamental group of $\mathbb{P}^1 - \{0, 1, \infty\}$," in *Arithmetic fundamental groups and noncommutative algebra (Berkeley, CA, 1999)*, vol. 70 of *Proc. Sympos. Pure Math.*, pp. 247–273. Amer. Math. Soc., Providence, RI, 2002.

[25] L. Schneps, "On the Poisson bracket on the free Lie algebra in two generators," *J. Lie Theory* **16** (2006) no. 1, 19–37.

[26] A. Pollack, "Relations between derivations arising from modular forms." https://dukespace.lib.duke.edu/dspace/handle/10161/1281, 2009. Undergraduate thesis, Duke University.

[27] F. Brown, "Zeta elements in depth 3 and the fundamental lie algebra of the infinitesimal tate curve," *Forum of Mathematics, Sigma* **5** (2017) , arXiv:1504.04737 [math.NT].

[28] A. B. Goncharov, "Multiple polylogarithms and mixed tate motives," arXiv:math/0103059 [math.AG].

[29] A. Goncharov, "Galois symmetries of fundamental groupoids and noncommutative geometry," *Duke Math.J.* **128** (2005) 209, arXiv:math/0208144 [math.AG].

[30] D. Zagier, "The Bloch-Wigner-Ramakrishnan polylogarithm function," *Math. Ann.* **286** (1990) 613.

[31] E. D'Hoker, M. B. Green, and B. Pioline, "Asymptotics of the $D^8\mathcal{R}^4$ genus-two string invariant," *Commun. Num. Theor. Phys.* **13** (2019) no. 2, 351–462, arXiv:1806.02691 [hep-th].

[32] A. Basu, "Poisson equations for elliptic modular graph functions," *Phys. Lett. B* **814** (2021) 136086, arXiv:2009.02221 [hep-th].

[33] E. D'Hoker, A. Kleinschmidt, and O. Schlotterer, "Elliptic modular graph forms. Part I. Identities and generating series," *JHEP* **03** (2021) 151, arXiv:2012.09198 [hep-th].

[34] M. Hidding, O. Schlotterer, and B. Verbeek, "Elliptic modular graph forms II: Iterated integrals," arXiv:2208.11116 [hep-th].

[35] B. Enriquez, "Flat connections on configuration spaces and braid groups of surfaces," *Advances in Mathematics* **252** (2014) 204–226, arXiv:1112.0864 [math.GT].

[36] B. Enriquez and F. Zerbini, "Construction of Maurer-Cartan elements over configuration spaces of curves," arXiv:2110.09341 [math.AG].

[37] B. Enriquez and F. Zerbini, "Analogues of hyperlogarithm functions on affine complex curves," arXiv:2212.03119 [math.AG].

[38] E. D'Hoker, M. Hidding, and O. Schlotterer, "Constructing polylogarithms on higher-genus Riemann surfaces," arXiv:2306.08644 [hep-th].

[39] E. D'Hoker and M. B. Green, "Zhang-Kawazumi Invariants and Superstring Amplitudes," *J. Number Theor.* **144** (2014) 111, arXiv:1308.4597 [hep-th].

[40] B. Pioline, "A Theta lift representation for the Kawazumi-Zhang and Faltings invariants of genus-two Riemann surfaces," *J. Number Theor.* **163** (2016) 520–541, arXiv:1504.04182 [hep-th].

[41] E. D'Hoker, M. B. Green, and B. Pioline, "Higher genus modular graph functions, string invariants, and their exact asymptotics," *Commun. Math. Phys.* **366** (2019) no. 3, 927–979, arXiv:1712.06135 [hep-th].

[42] A. Basu, "Eigenvalue equation for genus two modular graphs," *JHEP* **02** (2019) 046, arXiv:1812.00389 [hep-th].

[43] N. Kawazumi, "Lecture "Some tensor field on the Teichmüller space" given at MCM2016, OIST." https://www.ms.u-tokyo.ac.jp/~kawazumi/OIST1610_v1.pdf, 2016.

[44] N. Kawazumi, "Lecture "Differential forms and functions on the moduli space of Riemann surfaces" given in the "Séminaire Algèbre et topologie, Université de Strasbourg"." https://www.ms.u-tokyo.ac.jp/~kawazumi/1701Strasbourg_v1.pdf, 2017.

[45] E. D'Hoker and O. Schlotterer, "Identities among higher genus modular graph tensors," *Commun. Num. Theor. Phys.* **16** (2022) no. 1, 35–74, arXiv:2010.00924 [hep-th].

[46] N. Kawazumi, "A twisted invariant of a compact Riemann surface," arXiv:2210.00532 [math.GT].

[47] H. Furusho, "The multiple zeta value algebra and the stable derivation algebra," *Publ. Res. Inst. Math. Sci.* **39** (2003) no. 4, 695–720. http://projecteuclid.org/euclid.prims/1145476044.

[48] M. E. Hoffman, "Quasi-shuffle products," *J. Algebraic Combin.* **11** (2000) 49–68, arXiv:9907173v1.

[49] J. I. B. Gil and J. Fresan, "Multiple zeta values: from numbers to motives," *Clay Mathematics Proceedings,* to appear. http://javier.fresan.perso.math.cnrs.fr/mzv.pdf.

[50] M. E. Hoffman, "Multiple harmonic series," *Pacific J. Math.* **152** (1992) no. 2, 275–290. http://projecteuclid.org/euclid.pjm/1102636166.

[51] C. Duhr, "Hopf algebras, coproducts and symbols: an application to Higgs boson amplitudes," *JHEP* **08** (2012) 043, arXiv:1203.0454 [hep-ph].

[52] J. M. Drummond and E. Ragoucy, "Superstring amplitudes and the associator," *JHEP* **08** (2013) 135, arXiv:1301.0794 [hep-th].

[53] F. Brown and C. Dupont, "Single-valued integration and double copy," *J. Reine Angew. Math.* **2021** (2021) no. 775, 145–196, arXiv:1810.07682 [math.NT].

[54] F. Brown and C. Dupont, "Lauricella hypergeometric functions, unipotent fundamental groups of the punctured Riemann sphere, and their motivic coactions," *Nagoya Math. J.* **249** (2023) 148–220, arXiv:1907.06603 [math.AG].

[55] S. Abreu, R. Britto, and C. Duhr, "The SAGEX review on scattering amplitudes Chapter 3: Mathematical structures in Feynman integrals," *J. Phys. A* **55** (2022) no. 44, 443004, arXiv:2203.13014 [hep-th].

[56] C. R. Mafra and O. Schlotterer, "Tree-level amplitudes from the pure spinor superstring," *Phys. Rept.* **1020** (2023) 1–162, arXiv:2210.14241 [hep-th].

[57] F. Brown, "Motivic periods and the projective line minus three points," in *Proceedings of the ICM 2014*. 2014. arXiv:1407.5165 [math.NT]. https://api.semanticscholar.org/CorpusID:118359180.

[58] F. Brown, "Notes on motivic periods," *Commun. Number Theory Phys.* **11** (2017) no. 3, 557–655, arXiv:1512.06410 [math.NT].

[59] R. Lyndon, "Free differential calculus. IV: The quotient groups of the lower central series," *Annals of Math.* **68(2)** (1958) 81–95.

[60] A. I. Širšov, "On free Lie rings," *Mat. Sb. (N.S.)* **45(87)** (1958) 113–122.

[61] C. Reutenauer, *Free Lie algebras*, vol. 7 of *London Mathematical Society Monographs. New Series*. The Clarendon Press, Oxford University Press, New York, 1993. Oxford Science Publications.

[62] D. Perrin and G. Viennot, "A note on shuffle algebras," 1981. Unpublished note, personal communication.

[63] J. W. Milnor and J. C. Moore, "On the structure of Hopf algebras," *Ann. of Math. (2)* **81** (1965) 211–264.

[64] N. Bourbaki, *Lie groups and Lie algebras. Chapters 1–3*. Elements of Mathematics (Berlin). Springer-Verlag, Berlin, 1998. Translated from the French, Reprint of the 1989 English translation.

[65] T. T. Q. Le and J. Murakami, "Kontsevich's integral for the Kauffman polynomial," *Nagoya Math. J.* **142** (1996) 39–65.

[66] J. Blümlein, D. J. Broadhurst, and J. A. M. Vermaseren, "The Multiple Zeta Value Data Mine," *Comput. Phys. Commun.* **181** (2010) 582–625, arXiv:0907.2557 [math-ph].

[67] O. Schnetz, "HyperlogProcedures." https://www.math.fau.de/person/oliver-schnetz/, 2023. Maple procedures available on the homepage of the author.

[68] L. Schneps, "Double shuffle and Kashiwara-Vergne Lie algebras," *J. Algebra* **367** (2012) 54–74, arXiv:1201.5316 [math.QA].

[69] H. Tsunogai, "On some derivations of Lie algebras related to Galois representations," *Publ. Res. Inst. Math. Sci.* **31** (1995) no. 1, 113–134.

[70] H. Tsunogai, "The stable derivation algebras for higher genera," *Israel J. Math.* **136** (2003) 221–250.

[71] Y. Ihara, "Braids, Galois groups, and some arithmetic functions," in *Proceedings of the International Congress of Mathematicians, Vol. I, II (Kyoto, 1990)*, pp. 99–120. Math. Soc. Japan, Tokyo, 1991.

[72] D. Calaque, B. Enriquez, and P. Etingof, "Universal KZB equations: the elliptic case," in *Algebra, arithmetic, and geometry: in honor of Yu. I. Manin. Vol. I*, vol. 269 of *Progr. Math.*, pp. 165–266. Birkhäuser Boston, Boston, MA, 2009. arXiv:math/0702670.

[73] B. Enriquez, "Analogues elliptiques des nombres multizétas," *Bull. Soc. Math. France* **144** (2016) no. 3, 395–427, arXiv:1301.3042 [math.NT].

[74] J. Broedel, N. Matthes, and O. Schlotterer, "Relations between elliptic multiple zeta values and a special derivation algebra," *J. Phys.* **A49** (2016) no. 15, 155203, arXiv:1507.02254 [hep-th].

[75] P. Lochak, N. Matthes, and L. Schneps, "Elliptic multizetas and the elliptic double shuffle relations," *International Mathematics Research Notices* **2021** (2021) 695–753, arXiv:1703.09410 [math.NT].

[76] J.-G. Luque, J.-C. Novelli, and J.-Y. Thibon, "Period polynomials and Ihara brackets," *J. Lie Theory* **17** (2007) 229–239, arXiv:math/0606301 [math.CO,math.NT].

[77] A. Grothendieck and M. Raynaud, *Revêtements Étales et Groupe Fondamental (SGA1)*, vol. 224 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1971.

[78] Y. André, *Une introduction aux motifs (motifs purs, motifs mixtes, périodes)*, vol. 17 of *Panoramas et Synthèses [Panoramas and Syntheses]*. Société Mathématique de France, Paris, 2004.

[79] R. Hain, "Notes on the universal elliptic KZB connection," *Pure Appl. Math. Q.* **16** (2020) no. 2, 229–312, `arXiv:1309.0580 [math.AG]`.

[80] L. Schneps, "ARI, GARI, Zig and Zag: An introduction to Écalle's theory of multizeta values," `arXiv:1507.01534 [math.NT]`.

[81] E. Raphael and L. Schneps, "On linearised and elliptic versions of the Kashiwara-Vergne Lie algebra," `arXiv:1706.08299v1 [math.QA]`.

[82] J. Écalle, "Eupolars and their bialternality grid," *Acta Vietnamica* **40** (2015) 545–636.

[83] S. Baumard and L. Schneps, "On the derivation representation of the fundamental Lie algebra of mixed elliptic motives," *Ann. Math. Qué.* **41** (2017) no. 1, 43–62, `arXiv:1510.05549 [math.QA]`.

[84] D. Dorigoni, A. Kleinschmidt, and O. Schlotterer, "Poincaré series for modular graph forms at depth two. Part I. Seeds and Laplace systems," *JHEP* **01** (2022) 133, `arXiv:2109.05017 [hep-th]`.

[85] D. Dorigoni, A. Kleinschmidt, and O. Schlotterer, "Poincaré series for modular graph forms at depth two. Part II. Iterated integrals of cusp forms," *JHEP* **01** (2022) 134, `arXiv:2109.05018 [hep-th]`.

[86] F. Brown and A. Levin, "Multiple elliptic polylogarithms," `arXiv:1110.6917 [math]`.

[87] D. Zagier, "Periods of modular forms and Jacobi theta functions," *Invent. Math.* **104** (1991) no. 3, 449–465.